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Dynamics of Quantum Correlations

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Dynamics of Quantum Correlations

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Abstract

The main aim of this thesis is to study quantum dynamics, with a focus on irreversible, dissipative dynamics, by collecting repeated observations and arranging them to form a process. This leads to quantum states of extended models with some simplifying features. The models explored here are quantum spins on Fermionic lattices and chains of quantum spins. We focus in particular on the randomising properties of the dynamics.

The thesis begins by exploring the relation between the average von Neumann and Rényi entropies of integer orders for shift-invariant quasi-free Fermionic lattice systems. This then leads to an investigation into approximating the von Neumann entropy in terms of a combination of integer-order Rényi entropies and an estimate for the quality of such an approximation is given.

Later, a rather general technique is introduced to model a quantum system's dynamics on a semi-infinite half-chain of quantum spins. Here, bounds are given for the average entropy of the model system as well as a general scheme for computing the average Rényi entropy of integer order of such models.

Finally, the half-chain model is made explicit with the example of a simple qubit evolving under a thermalising dissipative dynamics. With this example, the integer-order Rényi entropies are explicitly calculated. By optimising over all possible choices of models, a model-independent expression for the average Rényi entropies is derived.

Beknopte samenvatting

In deze thesis bestuderen we hoofdzakelijk onomkeerbare, dissipatieve kwantummechanische tijdsevoluties. Dit gebeurt aan de hand van herhaalde waarnemingen die tot een proces geordend worden. Zo verkrijgen we toestanden met een bijzondere en eenvoudige structuur op een uitgebreid systeem. Twee soorten modellen komen hier aan bod: kwantumspinketens en Fermionische roostermodellen. We richten ons vooral op de stochastische aspecten van de dynamica's.

In het eerste deel van de thesis bestuderen we het verband tussen de gemiddelde von Neumann-entropie en de gemiddelde heeltallige Rényi-entropieën van translatie-invariante, quasi-vrije Fermion toestanden op een rooster. We onderzoeken hoe we, voor dergelijke systemen, de von Neumann entropie kunnen benaderen door lineaire combinaties van heeltallige Rényi-entropieën. Daarnaast verkrijgen we ook een afschatting voor zulk een benadering.

Vervolgens stellen we een algemene methode op om dissipatieve kwantumdynamica's te modelleren aan de hand van half-oneindige kwantumspinketens. We tonen aan dat er een modelonafhankelijke bovengrens is voor de gemiddelde entropieën en we ontwikkelen een algemene methode om de heeltallige Rényi-entropieën te berekenen.

Tenslotte passen we de algemene methode die we ontwikkelden toe op een eenvoudig systeem: één qubit onderworpen aan een thermaliserende tijdsevolutie. Voor dit systeem kunnen de heeltallige Rényi-entropieën van de systeemmodellen expliciet uitgerekend worden. We verkrijgen eveneens een model-onafhankelijke uitdrukking voor deze entropieën door te variëren over alle mogelijke modellen.

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Chapter 1

Introduction

Similar to the invention of the printing press, the discovery of electricity and magnetism has revolutionised the way society communicates and provides more efficient ways to process and store information. Previously, we were limited for the most part to storing information on paper in the form of hand-written or printed notes. Today, information is stored and processed digitally by encoding it into series of ones and zeroes, binary digits or bits, which are then stored electromagnetically.

The quest to develop means for denser storage, faster processing and more rapid communication of information has begun to approach the threshold of what is achievable with classical physics. As of now, transistor elements of integrated circuits can be manufactured which are of the order of tens of nanometres in size. At atomic length scales, quantum effects such as tunnelling begin to play a significant role.

An interesting question then naturally arises, "Can we harness these quantum phenomena to achieve better results?" The answer is, at least in theory, yes. Building on the foundations of classical information theory, the relatively new field of quantum information science seeks to explore novel applications of quantum mechanics to information processing and communication.

In classical computing, information is first encoded into binary and then the resulting bits are encoded into the physical state of some macroscopic object. This could be achieved by representing a zero or a one by the absence or presence of an electrical signal in a transistor, or, by the direction of alignment of magnetic domains pointing either up or down. Analogously, information may be encoded into the state of a quantum system.

1.1 Quantum mechanics

In quantum mechanics, a d-level physical system is associated with a d-dimensional Hilbert space $\mathcal{H}$ and states of this physical system are associated with normalised vectors, or wavefunctions, on $\mathcal{H}$. All vectors which correspond to the same state differ only by a complex phase-factor. P. Dirac introduced a convenient *bra-ket* notation for working with such vector spaces. Using this notation, a state vector is represented by the ket $|\psi\rangle \in \mathbb{C}^d$ and is postulated to contain all information pertaining to the corresponding physical state. Corresponding to every ket $|\psi\rangle$ is a bra $\langle\psi|$ via a dual-correspondence which is made explicit via the Riesz representation theorem. This gives us a way to write the inner product of two state vectors, $|\psi\rangle$ and $|\phi\rangle$, living on the same Hilbert space as $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$. The probability of finding some system in the state given by vector $|\phi\rangle$ after it is prepared in some initial state, with vector $|\psi\rangle$, is given by $|\langle\phi|\psi\rangle|^2$, where we assume that these vectors are normalised, $\langle\psi|\psi\rangle = \langle\phi|\phi\rangle = 1$.

A physical observable of the system is a linear transformation of $\mathbb{C}^d$. We will limit ourselves to consider only finite systems; all system observables form a set of bounded Hermitian operators on the Hilbert space, $\mathcal{B}(\mathcal{H})$. The eigenvalues of these operators correspond to real physical quantities associated with the observable and must therefore be real. All observables should be Hermitian operators. Concretely, for some eigenstate $|\alpha_i\rangle$ and observable A, we can write the eigenvalue equation

$$A|\alpha_i\rangle = a_i|\alpha_i\rangle, \tag{1.1}$$

where a_i are eigenvalues of the operator A with corresponding eigenvectors $|\alpha_i\rangle$. The expectation of some observable A for a system in some state with vector $|\psi\rangle$ is given by the inner product of $|\psi\rangle$ with $A|\psi\rangle$,

$$\langle A\rangle := \langle\psi|A\psi\rangle. \tag{1.2}$$

The time-evolution of state vectors of quantum systems is given by the Schrödinger equation,

$$\imath\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle, \tag{1.3}$$

where H is the system Hamiltonian operator.

A fundamental property of quantum mechanics is the superposition principle; if $|\psi\rangle$ and $|\phi\rangle$ are normalised state vectors of a quantum system system, then the normalised linear combination $w|\psi\rangle + z|\phi\rangle$ is again a valid state for some $w, z \in \mathbb{C}$ where $|w|^2 + |z|^2 = 1$. In other words, if we take any two valid states of a quantum system then their superposition is also a valid state. Conversely,

any arbitrary state vector $|\psi\rangle \in \mathcal{H}$ can be expanded as a linear sum of any set of orthonormal basis vectors which span $\mathcal{H}$,

$$|\psi\rangle = \sum c_i |\phi_i\rangle, \tag{1.4}$$

where the coefficients $c_i = \langle\phi_i|\psi\rangle$.

The states considered thus far, each of which having a corresponding state-vector or wavefunction, are called "pure states" and these are not the most general quantum states. We can also consider a probability distribution of pure states, given in terms of a density operator which can be expressed as a density matrix after choosing a basis.

For example, if we take a statistical mixture of n pure states $|\psi_i\rangle$ where each occurs with probability p_i, then we define this mixed state in terms of the density operator

$$\rho = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|. \tag{1.5}$$

If we choose some orthonormal basis $|e_i\rangle$ in $\mathcal{H}$, we can write this density operator as a matrix, the density matrix with elements

$$\rho_{ij} = \sum_k p_k \langle e_i|\psi_k\rangle\langle\psi_k|e_j\rangle. \tag{1.6}$$

Density operators have only positive eigenvalues. Moreover, they are positive Hermitian operators where the eigenvalues correspond to probabilities. The density operators, like the observables, are Hermitian, $\rho^\dagger = \rho$.

The expectation of some observable A on this mixture of pure states can then be expressed as

$$\langle A\rangle = \sum_{i=1}^{n} p_i \langle\psi_i|A\psi_i\rangle = \operatorname{Tr}\rho A. \tag{1.7}$$

The density matrix is not a quantum object in the strictest sense, it is a classical statistical mixture of pure quantum states and so must have trace one and non-negative eigenvalues. In other words, a mixed state given in terms of a density matrix expresses the classical uncertainty of which pure state the system is in. Unit trace is a consequence of conservation of probability and follows from

$$\operatorname{Tr}\rho = \sum_{ij} p_j \langle e_i|\psi_j\rangle\langle\psi_j|e_i\rangle \tag{1.8}$$

$$= \sum_j p_j = 1. \tag{1.9}$$

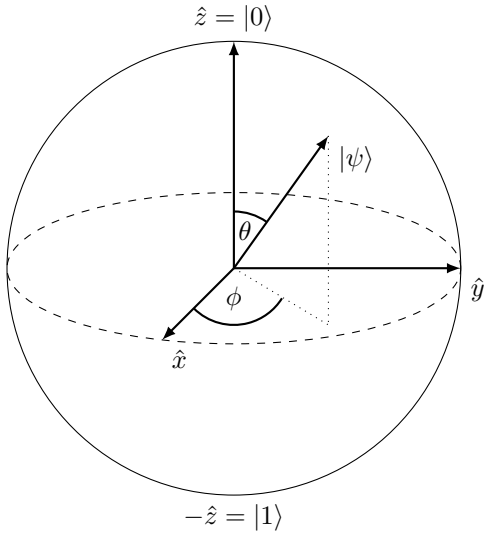

Figure 1.1: Bloch sphere depicting a general qubit state given in Equation (1.11).

For any given system, the set of all valid quantum states is a compact convex set. The pure states, which are the set of extreme points not expressible as a convex combination of any other states, lie on the topological boundary of this set of all states, although the boundary often also contains mixed states. The density operator of any pure state is a one-dimensional projector. A mixed state is some statistical mixture of pure states.

1.2 Qubit states

The simplest example of the state of a quantum system is the qubit, or quantum bit, represented as a vector in $\mathbb{C}^2$. It is the quantum analogue of the classical Ising spin - a state with only two possible configurations, "up" and "down".

Usually, one defines the standard basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1.10}$$

often referred to as the computational basis in the context of quantum information theory and quantum computing. A general qubit state vector

in $\mathbb{C}^2$ can be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)\exp(\imath\phi)|1\rangle, \tag{1.11}$$

where $\theta, \phi \in \mathbb{R}$, $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. This state can also be thought of as a point on the surface of a sphere of radius 1, as depicted in Figure (1.1).

A mixed state of a two-level system is given in terms of a two-dimensional density matrix. A common representation for qubit mixed states is given in terms of the Pauli matrices $\mathbb{1}, \sigma_x, \sigma_y, \sigma_z$ as

$$\rho = \frac{1}{2}\left(\mathbb{1} + x\sigma_x + y\sigma_y + z\sigma_z\right), \tag{1.12}$$

where $x, y, z \in \mathbb{R}$. Since the Pauli matrices σ_x, σ_y and σ_z are traceless, ρ automatically has trace one but positivity requires imposing the condition $x^2 + y^2 + z^2 \leq 1$.

As one might already have guessed, the pure state described by Equation (1.11) and depicted in Figure (1.1) corresponds to $(x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ and the state $|0\rangle$ depicted in Figure (1.1) corresponds to $(x, y, z) = (0, 0, 1)$.

1.3 Composite systems

If we are trying to describe two or more quantum systems, each with their own Hilbert space and which interact together, there is a way to describe them all together as a single quantum system living in a single Hilbert space. This is done through the use of the tensor product.

To illustrate this, suppose we have two quantum systems. System 1 lives on $\mathcal{H}_1$ and system 2 lives on $\mathcal{H}_2$. The tensor product of these two spaces is written as $\mathcal{H}_1 \otimes \mathcal{H}_2$ and it is this space on which the composite system lives. This composite space is built up by elements of the form $|\psi\rangle \otimes |\phi\rangle$ where $|\psi\rangle \in \mathcal{H}_1$ and $|\phi\rangle \in \mathcal{H}_2$. This is usually done by taking orthonormal sets of eigenvectors for each space, $\{|e_i\rangle \in \mathcal{H}_1\}$ and $\{|f_j\rangle \in \mathcal{H}_2\}$, and forming a set of basis vectors for the composite space by taking all possible combinations of $\{|e_i\rangle \otimes |f_j\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2\}$.

The inner product between elements in this tensor product space satisfy

$$\langle \phi_1 \otimes \psi_1 | \phi_2 \otimes \psi_2 \rangle = \langle \phi_1 \phi_2 \rangle \langle \psi_1 | \psi_2 \rangle \tag{1.13}$$

and the dimensions of these spaces are related by

$$\dim\left(\mathcal{H}_1 \otimes \mathcal{H}_2\right) = \dim\left(\mathcal{H}_1\right)\dim\left(\mathcal{H}_2\right). \tag{1.14}$$

These tensors are multilinear in their arguments, satisfying:

$$(|\psi_1\rangle + \alpha|\psi_2\rangle) \otimes |\phi\rangle = |\psi_1\rangle \otimes |\phi\rangle + \alpha\,(|\psi_2\rangle \otimes |\phi\rangle) \tag{1.15}$$

$$|\psi\rangle \otimes (|\phi_1\rangle + \alpha|\phi_2\rangle) = |\phi\rangle \otimes |\psi_1\rangle + \alpha\,(|\phi\rangle \otimes |\psi_2\rangle) \tag{1.16}$$

We are also able to restrict a state of the composite system to one of its subsystems. Consider the density matrix ρ_{12} of a bipartite state on a Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Suppose we wish to calculate an expectation on one of the subsystems. This is done by taking expectations of the form $\langle A\rangle_{\rho_1} = \langle A \otimes \mathbb{1}\rangle_{\rho_{12}}$ where $A \in \mathcal{B}(\mathcal{H}_1)$ or $\langle B\rangle_{\rho_2} = \langle \mathbb{1} \otimes B\rangle_{\rho_{12}}$ where $B \in \mathcal{B}(\mathcal{H}_2)$. This defines a connection between the full density matrix ρ_{12} and the reduced density matrices ρ_1 and ρ_2.

This connection is the partial trace - tracing not over the full composite space but only over certain subspaces. If $\{e_1, e_2, \ldots, e_m\}$ and $\{f_1, f_2, \ldots, f_n\}$ are orthonormal bases for $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively, then $\{e_i \otimes f_j\}$ is a basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$ where $i, j \in \mathbb{Z}$, $1 \leq i \leq m$ and $1 \leq j \leq n$.

We can then define a restricted density matrix ρ_1 on $\mathcal{H}_1$ as

$$\langle e_i|\rho_1|e_j\rangle = \sum_k \langle e_i \otimes f_k|\rho_{12}|e_j \otimes f_k\rangle. \tag{1.17}$$

This procedure is called a partial trace because we are tracing over all bases which do not lie in $\mathcal{H}_1$. It is not difficult to check that if ρ_{12} is positive with trace one, then both ρ_1 and ρ_2 will be positive with trace one.

1.4 Entanglement

When dealing with multipartite quantum systems, another phenomenon manifests itself which is not observable in classical systems - quantum entanglement. Entanglement exists when two or more quantum systems interact with each other or are created together in such a way that the quantum state of each individual system cannot be described independently. In 1935, A. Einstein, B. Podolsky and N. Rosen published a thought experiment leading to the so-called EPR paradox [21]. In this paper, they reason that the quantum state of two particles in a composite system cannot always be decomposed from the joint state of the pair.

Later, in 1964, J. Bell published results showing that the predictions made by quantum mechanics in the EPR experiment deviate significantly from those

of local hidden-variable theories [6]. This seemed to imply that when dealing with quantum systems, a much stronger statistical correlation is possible than is allowed in classical systems. These results have been repeatedly tested and verified; one of the earliest and most notable experiments was performed by a team led by A. Aspect in 1982 [4].

While classical pure states of multipartite systems can always be written as a product of pure states of their components, this is no longer generally true for quantum systems. As an example, consider the bipartite pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right). \tag{1.18}$$

The density matrix corresponding to this state is

$$\rho = \frac{1}{2}\left(|01\rangle + |10\rangle\right)\left(\langle 01| + \langle 10|\right) \tag{1.19}$$

$$= \frac{1}{2}\left(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|\right) \tag{1.20}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{1.21}$$

If we take the partial trace over the second subspace, we calculate that the density matrix of the first subsystem should be

$$\rho_a = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{1.22}$$

which is certainly not a pure state. Likewise, the density matrix of the second subsystem is calculated to be

$$\rho_b = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1.23}$$

As such, the composite density matrix in Equation (1.19) cannot be the result of a tensor product of two pure states. We say that the two subsystems a and b are *entangled* and cannot be described separately but instead can only be given by a single composite state.

States which are not entangled are called *separable*. Separable pure states can always be written in product form,

$$\rho = |\phi\rangle\langle\phi| = |\phi_1\rangle\langle\phi_1| \otimes |\phi_2\rangle\langle\phi_2|. \tag{1.24}$$

The state for any subsystem of a separable state can be recovered by taking the partial trace over the other subsystems,

$$\rho_1 = \mathrm{Tr}_2 \rho = |\phi_1\rangle\langle\phi_1| \tag{1.25}$$

and

$$\rho_2 = \mathrm{Tr}_1 \rho = |\phi_2\rangle\langle\phi_2|. \tag{1.26}$$

One can directly see that the product $\rho_1 \otimes \rho_2$ recovers the composite state.

An important result in characterising composite quantum systems is given by the Schmidt decomposition theorem.

Theorem 1 (Schmidt decomposition theorem)**.** *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces with dimensions n and m respectively, where $n \geq m$. For any vector $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ there exist orthonormal bases $e_1, \ldots, e_n \subset \mathcal{H}_1$ and $f_1, \ldots, f_m \subset \mathcal{H}_2$, the Schmidt bases, and a set of non-negative numbers $\{\alpha_1, \ldots, \alpha_m\}$, Schmidt coefficients, such that*

$$|\psi\rangle = \sum_{i=1}^{m} \alpha_i |e_i\rangle \otimes |f_i\rangle. \tag{1.27}$$

In the case of a normalised state where $\langle\psi|\psi\rangle = 1$, $\sum_{i=1}^{m} |\alpha_i|^2 = 1$.

The Schmidt bases can always be chosen such that the Schmidt coefficients are all real and non-negative. The number of non-zero Schmidt coefficients is called the Schmidt number and is uniquely defined for any given state $|\psi\rangle$.

A consequence of the Schmidt decomposition theorem, is that a composite state is entangled if and only if its Schmidt number is larger than one. Conversely, if the Schmidt number for a composite state is equal to one, then the state is separable. If the absolute values for all non-zero Schmidt coefficients are equal for an entangled composite system, then the system is said to be *maximally-entangled*.

Another consequence of the Schmidt decomposition theorem, is that the reduced density matrices $\rho_1 = \mathrm{Tr}_2 \rho$ and $\rho_2 = \mathrm{Tr}_1 \rho$ of a pure state of a composite system $\rho = |\psi\rangle\langle\psi|$ share the same eigenvalues up to multiplicities of zero. Such reduced states ρ_1 and ρ_2 are generally mixed states, and if $|\psi\rangle$ is maximally entangled, the reduced density matrices are proportional to the identities in the subspaces spanned by the Schmidt basis vectors belonging to the non-vanishing Schmidt coefficients. This is exactly what we saw with the example in Equation (1.18) with reduced density matrices given by Equations (1.22) and (1.23).

1.5 Entropy

Entropy is a measure of order/disorder of a system. In the context of information theory, it is the measure of uncertainty or predictability in a random variable and we usually speak of the Shannon entropy, introduced by C. Shannon [42] in his 1948 publication upon which much of today's classical information theory is founded. A good background to classical information theory can be found in [15].

Shannon entropy measures the average unpredictability of a random variable and is equivalent to its information content and is defined as

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log p(x_i), \tag{1.28}$$

where X is some random variable with outcomes $\{x_1, \ldots, x_n\}$ and $p(x_i)$ is the probability density function for the outcome x_i.

Two decades earlier, in 1927, J. von Neumann defined the von Neumann entropy of quantum states. Given as a function of some density matrix ρ, the von Neumann entropy is defined as

$$S(\rho) = -\mathrm{Tr}\, \rho \ln \rho, \tag{1.29}$$

and the von Neumann entropy of any pure state is zero while the entropy of any maximally mixed state on a Hilbert space of dimension d is just $\log d$.

The von Neumann entropy is equivalent to the Shannon entropy of the set of eigenvalues of ρ. Just as is the case with the Shannon entropy, the von Neumann entropy is also a concave function, such that

$$S(\lambda\rho_1 + (1-\lambda)\rho_2) \geq \lambda S(\rho_1) + (1-\lambda) S(\rho_2) \tag{1.30}$$

for any two states ρ_1 and ρ_2 where $0 \leq \lambda \leq 1$.

While the Shannon entropy enjoys many important properties, these do not always carry over to the quantum case. In 1970, H. Araki and E. Lieb proved some relations between entropies of reduced density matrices [3], including the so-called triangle inequality

$$|S(\rho_1) - S(\rho_2)| \leq S(\rho_{12}), \tag{1.31}$$

and in 1973 E. Lieb and M. Ruskai [32] proved the subadditivity and strong subadditivity properties of the von Neumann entropy for bipartite and tripartite quantum systems respectively.

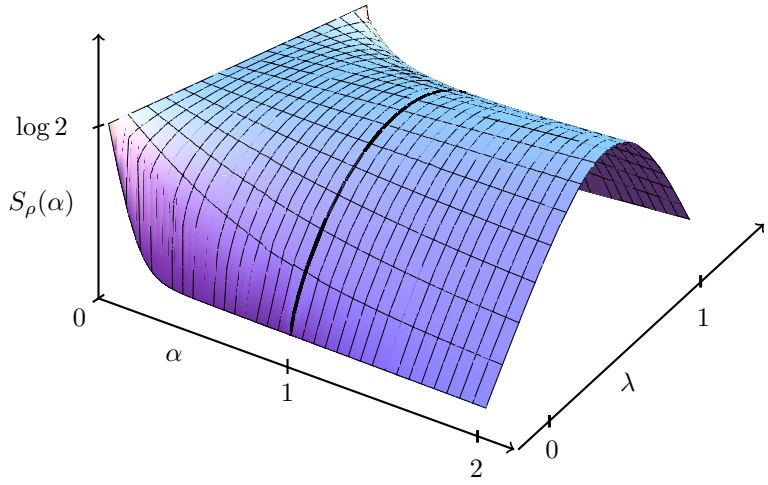

Figure 1.2: Rényi entropy $S_\rho(\alpha)$ of a 2-level system as a function of the order, α, and one of the two eigenvalues, λ. The thicker black band shows the von Neumann entropy limit at $\alpha \to 1$.

The strong subadditivity property states that the entropies of a tripartite quantum state ρ_{123} and its reduced states ρ_1, ρ_2 and ρ_3 are related by

$$S(\rho_{123}) + S(\rho_2) \leq S(\rho_{12}) + S(\rho_{23}). \tag{1.32}$$

In the case of a bipartite system with state ρ_{12}, this reduces to the subadditivity property

$$S(\rho_{12}) \leq S(\rho_1) + S(\rho_2). \tag{1.33}$$

As can be guessed from the (strong) subadditivity properties and Equations (1.18) to (1.23), the monotonicity property of the Shannon entropy does not carry over to the quantum case. This is because a composite pure state usually reduces to a mixed state when taking a partial trace because reduced subsystems of pure states usually share some entanglement, as we saw in Section (1.4).

In 1961, A. Rényi [39] introduced a generalised entropy of order α defined as

$$\mathsf{S}_\rho(\alpha) := -\frac{1}{\alpha - 1} \log \operatorname{Tr} \rho^\alpha, \tag{1.34}$$

where ρ is a density matrix, $\alpha \neq 1$, and $\alpha \geq 0$. The von Neumann entropy is a special case of the Rényi entropy, obtained in the limit

$$\mathsf{S}_\rho = \lim_{\alpha \to 1} \mathsf{S}_\rho(\alpha) = -\operatorname{Tr} \rho \log \rho. \tag{1.35}$$

Rényi entropies of integer order $\alpha \in \{2, 3, \ldots\}$ are easily computed: one only needs matrix multiplication and taking the trace. For fractional orders or for the von Neumann entropy one should, in principle, diagonalise the density matrix which is a much harder problem.

The Rényi entropy, as depicted in Figure (1.2), is non-negative and monotonically decreasing in α[5]. The Rényi entropy for all orders is unitarily invariant and is zero for any pure state while being maximised for the maximally mixed state. The Rényi entropy is additive for product states, but subadditivity fails in general.

1.6 Chains and average entropies

In some situations, it can be useful to model a system by using a chain. A chain is built by connecting individual sites together such that translations along the chain represent discrete steps in either time or space.

Stochastic processes, for example, can be conveniently represented on a chain where the sites, each separated in time by a finite time-step Δt, represent the state of a system at some time. If the state of the system after i time-steps depends only on the state of the previous site, after $(i-1)$ time-steps, we say that the stochastic process is Markovian.

Although Markov processes are not the focus of this thesis, they are much easier to work with and are used here as a simple example of a process on a chain.

A translation-invariant Markov process is defined by a k-dimensional right-stochastic matrix T, called a transition matrix, with entries T_{ij} giving the probability to jump from state i to state j. The state is labelled by an element of the set $\{1..k\}$, while the probability of the system to be found in each of the k states is given by the probability vector

$$\mathbf{p} = (p_1, \ldots, p_k)\,. \tag{1.36}$$

The stationary distribution for such a process, $\boldsymbol{\mu}$, is the left-eigenvector of the transition matrix corresponding to eigenvalue 1.

Beginning in some initial state $\boldsymbol{\sigma}$ at time $t = 0$, the ith site on the chain is given by

$$\boldsymbol{p}_i = T^i \boldsymbol{\sigma}, \tag{1.37}$$

where $\boldsymbol{p}_i$ is the state of the system after i time-steps.

Instead of calculating the entropy of a system at any given time, one might wish to know the asymptotic behaviour of the system as we step forward in time. Entropy is an extensive property which grows with the system's volume. If we calculate the entropy of the entire chain of length n, that is an n-site chain containing the states of the system after each time-step, and divide by the number of sites we can calculate the average entropy per site. In the limit that the number of sites approaches infinity, this average entropy gives a measure of the randomising behaviour of the underlying process,

$$s(\rho) = \lim_{n\to\infty} \frac{1}{n} S(\rho_n), \tag{1.38}$$

where $\rho = \lim_{n\to\infty} \rho_n$ and ρ_n is the density matrix corresponding to the n-site chain.

The average Rényi entropy for a Markov process as described above is given by

$$\begin{aligned} s_T(\alpha) &= \lim_{n\to\infty} \frac{1}{n(1-\alpha)} \log\langle \boldsymbol{\mu}, (T^{\circ\alpha})^{n-1} \mathbb{1}\rangle & (1.39)\\ &= \frac{1}{1-\alpha} \log \rho(T^{\circ\alpha}), & (1.40) \end{aligned}$$

where $\rho(T^{\circ\alpha})$ is the spectral radius of the α-Hadamard power of the transition matrix. The Hadamard-product is just the element-wise product, given as

$$[A \circ B]_{ij} = [A]_{ij}[B]_{ij}. \tag{1.41}$$

By extension, the Hadamard power of some matrix A has entries

$$[A^{\circ n}]_{ij} = [A]_{ij}^n. \tag{1.42}$$

Here, we are taking n to be a natural number but for transition matrices, where every entry is positive, the Hadamard power may also be fractional.

The Shannon, or von Neumann, entropy is the limit of the Rényi entropy as $\alpha \to 1$,

$$s_T = -\sum_{i,j=1}^{k} \mu_i T_{ij} \log T_{ij}. \tag{1.43}$$

1.7 Systems with variable particle number

The elementary building blocks of matter are the Fermions, while interactions between matter constituents is mediated by Bosons. These two classes of elementary particles obey very different statistics, namely, Fermi-Dirac in the case of Fermions and Bose-Einstein in the case of Bosons.

When building models of Fermionic systems, in order to describe some particular phenomenon for example, one can often neglect the interactions between particles and still have a meaningful model. This is because in certain systems the general behaviour of their constituents is governed by their statistics. An example of such a case is when looking at the free-electron model in crystalline metallic solids. Systems of non-interacting fermions can provide a model which is both manageable and useful, leading to good approximations of real systems. In preparation for what is to come in Chapter (2), we will go over some of the basic tools and notations used in describing finite quasi-free Fermionic systems.

If we have a system of two independent indistinguishable particles, labelled 1 and 2, their composite state can be equally described by either $|\phi_1\rangle \otimes |\phi_2\rangle$ or $|\phi_2\rangle \otimes |\phi_1\rangle$. The composite pure state vector is therefore written as

$$|\phi_\pm\rangle \approx |\phi_1\rangle \otimes |\phi_2\rangle \pm |\phi_1\rangle \otimes |\phi_2\rangle, \tag{1.44}$$

where the proportionality constant is $1/\sqrt{2}$ if the vectors $|\phi_1\rangle$ and $|\phi_2\rangle$ are mutually orthogonal.

The $+$ states, $|\phi_+\rangle$, are symmetric under particle exchange and are called Bosonic. Likewise, the $-$ states, $|\phi_-\rangle$, are antisymmetric under particle exchange and are called Fermionic.

For Fermionic systems of a number of indistinguishable particles, every interchange of a particle pair in the system results in the composite state picking up a factor -1. If the system exists in some permutation σ, we express the number of pairwise particle exchanges for that configuration as $\epsilon(\sigma)$. In this way, we can write the general state for a system of n Fermions as

$$|\phi_1\rangle \wedge \cdots \wedge |\phi_n\rangle = \frac{1}{\sqrt{n!}} \sum_\sigma \epsilon(\sigma) |\phi_{\sigma(1)}\rangle \otimes |\phi_{\sigma(2)}\rangle \otimes \cdots \otimes |\phi_{\sigma(n)}\rangle, \tag{1.45}$$

where $\wedge$ represents the antisymmetric tensor product and the sum is taken over all $n!$ possible permutations of the configurations σ. The space formed by these antisymmetric vectors is expressed as

$$\mathcal{H}^{\wedge n} = \underbrace{\mathcal{H} \wedge \cdots \wedge \mathcal{H}}_{n \text{ times}}. \tag{1.46}$$

$$\mathcal{H}^{\otimes_{AS}^{n}} = \underbrace{\mathcal{H} \otimes_{AS} \cdots \otimes_{AS} \mathcal{H}}_{n \text{ times}}. \tag{1.47}$$

The structure of this space lends itself well to describing systems of multiple particles because, by ignoring interactions and having free Fermions, everything is determined by the single-particle Hamiltonian, the single-particle Hilbert space $\mathcal{H}$ and Fermi-Dirac statistics.

The Fermionic Fock space, named after V. Fock [25], is the direct sum over particle number n,

$$\mathcal{F}(\mathcal{H}) = \mathbb{C} \oplus \mathcal{H} \oplus (\mathcal{H} \wedge \mathcal{H}) \oplus \cdots = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\wedge n}. \tag{1.48}$$

This Fock space describes the state of a system of indeterminate particle number; each term in the sum from Equation (1.48) corresponds to a definite number of particles with $\mathbb{C}$ being the empty state with no particles and we can write the *vacuum state* as $\Omega := 1 \oplus 0 \oplus \ldots$.

The number of particles in a particular state, or mode, can be raised or lowered through the use of the so-called creation of annihilation operators a^* and a respectively. For a system of n particles,

$$a^*(\psi)\left(\phi_1 \wedge \cdots \wedge \phi_n\right) = \psi \wedge \phi_1 \wedge \cdots \wedge \phi_n \tag{1.49}$$

and

$$a(\psi)\left(\phi_1 \wedge \cdots \wedge \phi_n\right) = \sum_{i=1}^{n} (-1)^i \langle \psi | \phi_i \rangle \left(\phi_1 \wedge \cdots \wedge \phi_{i-1} \wedge \phi_{i+1} \wedge \cdots \wedge \phi_n\right). \tag{1.50}$$

The operators a^* and a satisfy the anticommutation relations

$$\{a(\psi), a(\phi)\} = 0 \text{ and } \{a(\psi), a^*(\phi)\} = \langle \psi | \phi \rangle \mathbb{1}. \tag{1.51}$$

These relations are known as the canonical anticommutation relations (CAR). Every bounded linear operator on the Fock space $\mathcal{F}(\mathcal{H})$ is generated by the creation and annihilation operators, a^* and a respectively, and the identity $\mathbb{1}$; the abstract algebra defining the behaviour of these operators is called the CAR-algebra $\mathcal{A}(\mathcal{H})$.

A free state ω_Q on $\mathcal{A}(\mathcal{H})$ is determined by the symbol Q, a bounded, positive, linear operator on $\mathcal{H}$ where $0 \leq Q \leq \mathbb{1}$, such that

$$\omega_Q(\mathbb{1}) = 1 \tag{1.52}$$

and

$$\omega_Q(a^*(\phi_1)\dots a^*(\phi_m)a(\psi_n)\dots a(\psi_1)) := \delta_{m,n}\det\left([\langle\psi_i, Q\ \phi_j\rangle]_{i,j}\right). \quad (1.53)$$

The set of all symbols forms a convex set where the extreme points (orthogonal projectors) correspond to pure free states.

Quantities such as the entropy of free states of Fermionic systems can be expressed in terms of their corresponding symbol Q; the von Neumann entropy being

$$S_Q = -\mathrm{Tr}\, Q\log Q - \mathrm{Tr}\ (\mathbb{1}-Q)\log(\mathbb{1}-Q) \quad (1.54)$$

while the α-order Rényi entropy is expressed as

$$S_Q(\alpha) = \frac{1}{1-\alpha}\mathrm{Tr}\ \log\left((\mathbb{1}-Q)^\alpha + Q^\alpha\right). \quad (1.55)$$

The symbol Q is not a density matrix and its trace is equal to the total particle number. The symmetry between Q and $\mathbb{1}-Q$ is a result of particle-hole symmetry. The density matrix corresponding to the state ω_Q can be expressed in terms of Q. More details can be found in [12, 19].

1.8 Outlook

This chapter has introduced to the reader the foundational concepts necessary for following and understanding the work in the chapters to come. For some readers, this introduction serves as a reminder of the basics of quantum mechanics but for those encountering these topics for the first time there exist many excellent books one may refer to in order to get a more complete understanding [14, 40, 41].

Chapter (2) explores the connection between the von Neumann and Rényi entropies. As mentioned here in this introduction, the von Neumann entropy is just the limit of the Rényi entropy as the order tends to one. However, it is not always feasible to work with von Neumann entropies in practice since diagonalising large-dimensional density matrices often proves to be an intractable problem. On the other hand, it is often comparatively easy to calculate integer-order Rényi entropies for these systems. In Chapter (2), it is shown that it is possible to approximate the von Neumann entropy of a quasi-free Fermionic system on a lattice given a number of integer-order Rényi entropies. An approximation scheme is presented and explicit examples are given.

Chapter (3) introduces the concept of dynamics in quantum systems and describes some of the difficulties in characterising the entropies of such systems. The notion of the generalised pointer measurement is introduced and is used to build up a model of multi-time correlations for a general n-level quantum system in the form of a spin-chain. Using this spin-chain model, it is shown that the problem of calculating the amount by which the Rényi entropy increases by adding a site to the chain, in the limit that the chain becomes semi-infinite, is equivalent to finding the largest eigenvalues of a matrix corresponding to both the dynamics and the system in question.

While this technique of modelling systems and characterising their dynamical Rényi entropies is completely general, it still poses the challenge of being a high-dimensional eigenvalue problem as the dimensions of the system of interest grows. Nonetheless, some general bounds on entropic growth rates are calculated and numerical techniques remain quite useful. Chapter (4) presents an explicit example in the form of a two-level system. In this case, the problem of finding the second-order average Rényi entropy is still exactly solvable.

Chapter 2

Connecting Rényi and von Neumann entropies

In the previous chapter, the basic ideas behind quantum information and quantum systems were introduced. Specifically, the idea of entropy and its role in characterising information in the context of quantum systems was outlined. In Section (1.5), a number of different entropies were defined, each one playing a part in describing the information content of quantum systems. There are many other definitions of entropy, some of which have quite different properties when compared to the more commonly-used von Neumann entropy, such as the Tsallis entropy, relative entropy, etc.

Given its central role in quantum information, the motivation for this chapter is to better understand the relation between the average von Neumann entropy and the average Rényi entropies of integer order. Entropies are non-local characteristics of a state and are, to give an example, an essential input in maximal entropy principles such as the variational principle for thermal equilibrium. Restricting the variational principle to specific classes of states leads to well-known approximations including mean-field and Hartree-Fock [34]. More refined approximation schemes such as using matrix product states for computing ground states of quantum spin chains have turned out to be quite effective [28, 37]. Extensions to higher dimensional quantum spin lattices are currently being investigated [23] and one might wonder about using general finitely correlated states for thermal states. Computing the average von Neumann entropy for a general, shift-invariant, finitely correlated state is, however, still an open problem [24].

The entropy of a d-dimensional quantum system where d is finite is always bounded. The lower-bound is of course zero and is achieved when the state of the system is pure. In this case, the corresponding density matrix has only a single non-zero eigenvalue which is equal to one. The upper-bound is saturated when all of the d eigenvalues are equal, each being equal to $1/d$. In this case, the distribution of states is uniform and the entropy is equal to $-\log(d)$. As such, for any general d-dimensional density matrix, its entropy obeys the bound

$$0 \leq S(\rho) \leq \log(d). \tag{2.1}$$

For very large systems, one may argue that a uniform distribution of states is a reasonable approximation, and for such systems in equilibrium the entropy gives some idea of the dimensionality of the relevant part of the density matrix. Though, in general, one should not expect every equilibrium state to be tracial. When considering ground states, the entropy of their reduced density matrices usually grow with volume, since entropy is an extensive property. In fact, for ground states in lattice-systems where the interaction-distance is short, the entropy of the reduced density operator ρ_A corresponding to some region A is proportional to the surface boundary of that region [30, 46].

It is because of the relative difficulty in computing the von Neumann entropy, and the ease with which one can compute an integer-order Rényi entropy, that we find value in exploring the connection between these two.

Let us first look back to Equation (1.34), where we introduced Rényi's generalised entropy of order α defined as

$$\mathsf{S}_\rho(\alpha) := -\frac{1}{\alpha - 1} \log \operatorname{Tr} \rho^\alpha, \tag{2.2}$$

where ρ is a density matrix, $\alpha \neq 1$, and $\alpha \geq 0$. The von Neumann entropy is recovered as a special case in the limit

$$\mathsf{S}_\rho = \lim_{\alpha \to 1} \mathsf{S}_\rho(\alpha) = -\operatorname{Tr} \rho \log \rho. \tag{2.3}$$

For integer orders, it is often convenient to express the Rényi entropy in terms of several copies of the system. This is called the replica trick:

$$\operatorname{Tr} \rho^n = \operatorname{Tr} \left(\underbrace{\rho \otimes \rho \otimes \cdots \otimes \rho}_{n \text{ times}} \, T_n \right) \tag{2.4}$$

where T_n is the cyclic shift on the n-fold tensor power of the original system:

$$T_n \big(\varphi_1 \otimes \varphi_2 \otimes \cdots \otimes \varphi_n \big) = \varphi_2 \otimes \cdots \otimes \varphi_n \otimes \varphi_1. \tag{2.5}$$

Formula (2.4) can be checked by evaluating its right-hand side in a tensor basis:

$$\begin{aligned}\operatorname{Tr}\rho\otimes\rho\otimes\cdots\otimes\rho T_n &= \sum_{i_1,\dots,i_n}\left\langle e_{i_1}\otimes\cdots\otimes e_{i_n}, \rho\otimes\cdots\otimes\rho T_n\, e_{i_1}\otimes\cdots\otimes e_{i_n}\right\rangle\\ &= \sum_{i_1,\dots,i_n}\left\langle e_{i_1}\otimes\cdots\otimes e_{i_n}, \rho\otimes\cdots\otimes\rho\, e_{i_2}\otimes\cdots\otimes e_{i_1}\right\rangle\\ &= \sum_{i_1,\dots,i_n}\langle e_{i_1}, \rho\, e_{i_2}\rangle\langle e_{i_2}, \rho\, e_{i_3}\rangle\cdots\langle e_{i_n}, \rho\, e_{i_1}\rangle\\ &= \operatorname{Tr}\rho^n. \end{aligned} \tag{2.6}$$

For an example of this replica trick applied to a spin glass see [18], for an example of the replica trick applied to the compution of an average Rényi entropy see [24]. Apart from the obvious application in statistical mechanics, Rényi entropies are also used in the analysis of multiparticle states produced in high-energy collisions, see e.g., [9] and [10]. Rényi entropies are also of interest in the context of catalysis in quantum information theory. The question that inspired this work is whether it is possible to reconstruct the von Neumann entropy given the Rényi entropies of integer order $2, 3, \dots$ and, if so, how to do this.

In fact, the relevant quantity for shift-invariant states is the average Rényi entropy. Unfortunately, these densities pose several serious problems with regard to existence and continuity. In general, they simply don't exist and they are also not affine on convex subsets of shift-invariant states. Their use is therefore limited to states with strong clustering. Moreover, it is completely unclear whether, in general, the knowledge of integer-order average Rényi entropies uniquely determines the average von Neumann entropy.

A number of papers have considered relations between the integer-order Rényi and von Neumann entropies [29, 27, 47]. These relations don't always scale properly with the system size and therefore don't necessarily survive on the level of densities. There is certainly no general procedure, even under strong assumptions on clustering, for passing from integer-order Rényi to von Neumann entropies. Further suggested reading on the subject can be found in [7, 36, 38].

In this chapter, we consider the case of shift-invariant quasi-free Fermionic states on a lattice. We show that such a reconstruction procedure exists in this case and obtain some simple approximations in terms of the first few Rényi densities.

The chapter is organised as follows: in Section 2.3, we remind the reader of the description of Fermions on a lattice and introduce some notation. Section 2.4

gives the expression for the average Rényi entropies of quasi-free states. In Section 2.5, we introduce a completely monotonic entropy function which is then used in Section 2.6 to reconstruct the von Neumann entropy. Finally, we provide an explicit approximation scheme in Section 2.7.

2.1 A non-linear reconstruction

For any arbitrary finite-dimensional density matrix $\rho \in \mathcal{M}^d$, we can usually expect to be able to fully recover every eigenvalue if we are given sufficiently many integer-order Rényi entropies of the unknown state corresponding to ρ.

To demonstrate this, consider an example of a three-level system for which we are given two Rényi entropies. We can write the corresponding, as-yet unknown, density matrix as

$$\rho = \begin{pmatrix} 1-a-b & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix}. \tag{2.7}$$

We are then given the Rényi entropies

$$S_2(\rho) = \log \frac{1225}{603} \quad \text{and} \quad S_3(\rho) = \log \frac{35}{19}. \tag{2.8}$$

This information along with Equation (2.2) is sufficient to determine the two free parameters a and b. We find that

$$\lambda_1 = \frac{1}{7}, \ \lambda_2 = \frac{1}{5} \quad \text{and} \quad \lambda_3 = \frac{23}{35}. \tag{2.9}$$

The following second example concerns itself with a dynamical process. Suppose that a Markov process on a d-dimensional system is defined by a d-dimensional transition matrix,

$$\begin{pmatrix} t_{1,1} & t_{1,2} & \cdots & t_{1,d} \\ t_{2,1} & t_{2,2} & \cdots & t_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ t_{d,1} & t_{d,2} & \cdots & t_{d,d} \end{pmatrix}, \tag{2.10}$$

where $0 \leq t_{i,j} \leq 1$ and $\sum_{i=1}^{d} t_{i,j} = 1$. This leaves $d^2 - d$ free parameters defining the matrix.

Furthermore, suppose we have knowledge of the largest eigenvalue of $T^{\circ k}$ for some set of integers:

k	$\rho(T^{\circ k})$
2	$\rho(T^{\circ 2})$
3	$\rho(T^{\circ 3})$
$\vdots$	$\vdots$
n	$\rho(T^{\circ n})$

where we recall that the Hadamard product of two matrices X and Y is taken as the element-wise product

$$[X \circ Y]_{ij} = [X]_{ij}[Y]_{ij},$$

and, following from this, the Hadamard power can be written

$$[X^{\circ k}]_{ij} = [X]_{ij}^{k}.$$

For any matrix M, the equation

$$\sum_{i=0}^{d}(-1)^{i}\sum_{j=1}^{d-i} M_{j,i}\lambda^{d-i} = 0 \tag{2.11}$$

where $M_{j,i}$ is the i-th principal minor of the transition matrix T is satisfied if λ is any eigenvalue of T. We can use this to find a relation between the transition matrix T and the spectral radius of $T^{\circ k}$ for each k.

Consider the specific example of a two-dimensional transition matrix defining some Markov process,

$$T = \begin{pmatrix} 1-x & x \\ y & 1-y \end{pmatrix}, \tag{2.12}$$

together with information about the spectral radius of $T^{*\alpha}$ for a number of integer Hadamard exponents α:

α	$\rho(T^{\circ\alpha})$
2	0.50737
3	0.261272

Using this information, we can write the following two expressions from Equation (2.11):

$$\begin{aligned} \lambda_2^2 - \lambda_2((x-1)^2 + (y-1)^2) + (x-1)^2(y-1)^2 - x^2y^2 &= 0 \\ \lambda_3^2 - \lambda_3((x-1)^3 + (y-1)^3) + (x-1)^3(y-1)^3 - x^3y^3 &= 0, \end{aligned}$$

where $\lambda_i = \rho(T^{\circ i})$. Solving these two equations simultaneously, one finds that the two solutions intersect not just once, but twice. Choosing the correct one of these two sets of solutions requires further information. Indeed, if one is presented with the additional point $\rho(T^{\circ\alpha}) = 0.136584$ when $\alpha = 4$, the set of solutions narrows to one, giving the result $x = 3/7$ and $y = 5/11$.

Knowledge of enough Rényi entropies is almost always sufficient to fully reconstruct the entire density matrix in the first example, or transition matrix in the second although one may require a large number of entropies due to the high non-linearity. However, solving such problems rapidly becomes very difficult as the dimensions grow due to the non-linearity of the set of simultaneous equations. This makes such a technique rather undesirable and will not be the approach used in this chapter. Instead, a linear approximation scheme will be constructed which can achieve arbitrary precision given enough integer-order Rényi entropies.

2.2 A linear approximation using product states

Rather than an often intractable non-linear reconstruction, let us explore the idea of a linear approximation with the help of a fairly simple example. Here, we will construct an approximation of the von Neumann entropy density for an n-site chain in terms of a set of integer-order Rényi entropies.

In this example, we assume that the state of the infinite chain is a product state composed of independent, identical single-site states. This simplifies things somewhat because the von Neumann or Rényi entropy density is just equal to the single-site entropy,

$$s_\rho = S_{\rho_1} \quad \text{and} \quad s_\rho(\alpha) = S_{\rho_1}(\alpha), \tag{2.13}$$

where the state of the whole chain, ρ, is given as

$$\rho = \otimes^{\mathbb{N}} \rho_1. \tag{2.14}$$

The n-site reduced density matrix can then be expressed as

$$\rho_n = \otimes^n \rho_1. \tag{2.15}$$

The objective now is to make the k-term approximation

$$f_k(\rho) = \sum_{i=2}^{k} c_i s_i(\rho) \tag{2.16}$$

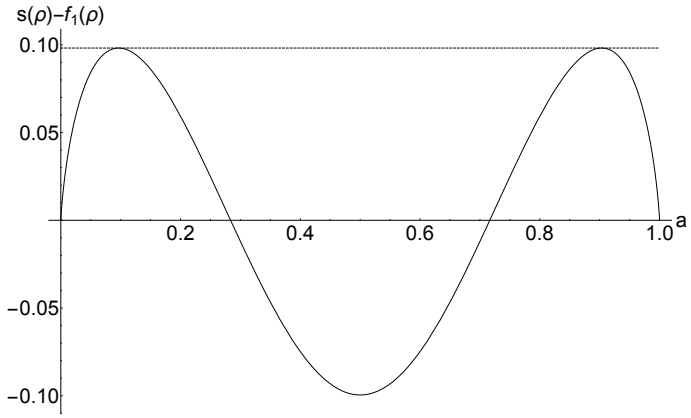

Figure 2.1: Plot of $s_\rho - cs_\rho(2)$ for $c = 1.14$ as a function of the parameter a determining ρ_1, bearing in mind that $\max s_{\rho_1} = \log 2$. The extrema are equal in magnitude to 0.0982.

given a set of k integer-order average Rényi entropy densities $\{s_i(\rho) \,|\, i \in \mathbb{N}, 2 \leq i \leq k\}$, and optimise it by minimising the error over all coefficients $\{c_i\}$:

$$\min_{\{c_i\}} \sup_{\rho} \left\{ \left| s_{\rho_1} - \sum_{i=2}^{k} c_i s_{\rho_1}(i) \right| \right\} \tag{2.17}$$

As an example, consider the qubit with density matrix

$$\rho_1 = \begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix}. \tag{2.18}$$

Let us begin with the simplest case, a single-term approximation using the second-order Rényi entropy $s_2(\rho)$. We can then write

$$f_1(\rho) = cs_2(\rho) = -c \log \operatorname{Tr} \rho^2, \tag{2.19}$$

and express the difference with the von Neumann entropy as

$$s(\rho) - cs_2(\rho). \tag{2.20}$$

Taking the sup-norm over ρ and minimising with respect to c, we find that the worst-case error, $\sup_\rho\{|s(\rho) - f_1(\rho)|\}$, is minimised when $c = 1.144$, as shown in Figure(2.1). This yields a maximum error of around 14.0%, or 0.0982.

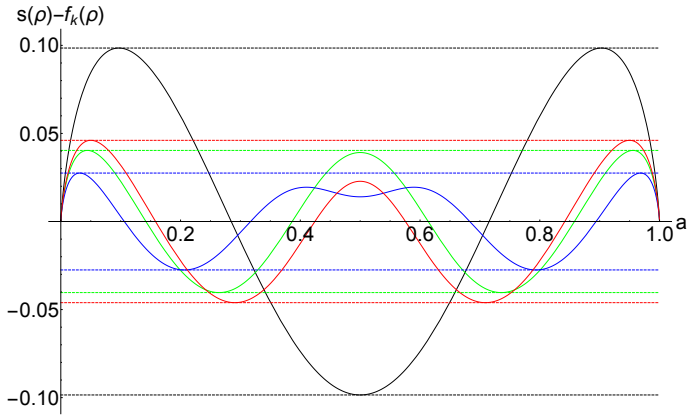

Figure 2.2: Plot of optimal approximation errors $s(\rho) - f_i(\rho)$as a function of the parameter a determining ρ, bearing in mind that $\max s(\rho) = \log 2$. The one-term approximation in black has a maximum of 0.098, the two-term in green has a maximum of 0.040 and the three-term in blue has a maximum of 0.035.

Continuing in the same fashion, the two-term approximation using the second and third-order Rényi entropies we find that

$$s(\rho) - c_2 s_2(\rho) - c_3 s_3(\rho) \tag{2.21}$$

is optimised when $c_2 = 3.753$ and $c_3 = -2.811$, giving a maximum error of 0.0402, or around 5.8%, a good improvement over the single-term approximation.

Likewise, the three-term approximation, $f_3(\rho)$ is optimal when $c_2 = 4.725$, $c_3 = -6.230$ and $c_4 = 2.507$ with a maximum error of 0.0349, or around 5.0%. The single, two and three-term approximation errors are found in Figure (2.2).

The four-term approximation, $f_4(\rho) = s(\rho) - c_2 s_2(\rho) - c_3 s_3(\rho) - c_4 s_4(\rho) - c_5 s_5(\rho)$, is optimal when $c_2 = 4.725$, $c_3 = -6.230$, $c_4 = 2.507$ and $c_5 = 0$ with a maximum error of 0.0349, or around 5.0%.

Here, we notice something a little different; the four-term approximation is certainly no better than the three-term. It could perhaps be a poor choice to use Rényi entropies of integer order 2, 3, 4, etc. to approximate the von Neumann entropy in this example. To see if it's possible to do better, one might decide to use entropies of order $0 < \alpha < 1$ in addition to integer-order in searching for a better approximation.

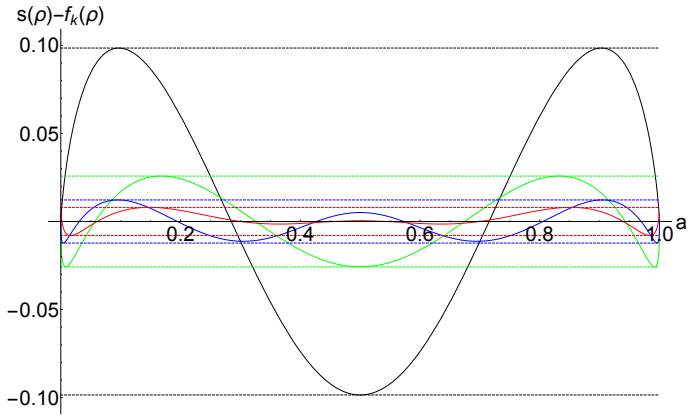

Figure 2.3: Plot of optimal approximation errors as a function of the parameter a determining ρ for f_1 in black, f_2 in green, f_3 in blue and f_4 in red. The functions $\{f_k(\rho)\}$ and their corresponding $\{c_i\}$ are given in Table (2.1).

f_k	c_1	c_2	c_3	c_4	Max error
$c_1 s_2$	1.142	/	/	/	0.0985
$c_1 s_2 + c_2 s_{\frac{1}{2}}$	0.660	0.377	/	/	0.0258
$c_1 s_2 + c_2 s_{\frac{1}{2}} + c_3 s_3$	1.885	0.253	−1.146	/	0.0122
$c_1 s_2 + c_2 s_{\frac{1}{2}} + c_3 s_3 + c_4 s_{\frac{1}{3}}$	1.07	0.714	−0.508	−0.278	0.00795

Table 2.1: Table of k-term linear approximations of the von Neumann entropy in terms of fractional and integer-order Rényi entropies.

Allowing the use of Rényi entropies of order i as well as $1/i$, where $i \in \mathbb{N} > 1$, indeed gives a much better approximation. Figure (2.3) shows this improved approximation for up to four terms, where a rather large decrease in the maximum error can be seen in comparison with Figure (2.2).

This linear approximation technique is more in line with what we hope to achieve in this Chapter. However, the improved approximation presented in Figure (2.3) is not strictly in the spirit of this chapter, since it requires taking fractional-order Rényi entropies involving n-th roots of the density matrix. The motivation for this technique was built around the ease of calculating integer-order Rényi entropies and so the reader should be cautioned that the example presented above is either suboptimal, in the case of integer orders, or computationally expensive, for fractional orders.

In either case, it is a non-trivial problem to correctly pick which order Rényi entropies to use in the approximation as this greatly influences its accuracy. Instead, if we recast the entropy densities in a form more amenable to approximating functions we can hope to achieve better results. The modification which will aid in this pursuit in the coming sections is using the Stone-Weierstrass theorem together with a Fourier transform.

2.3 Fermions on a lattice

Consider a system of Fermions living on some Bravais lattice $\mathcal{L}$ in $\mathbb{R}^d$:

$$\mathcal{L} = \{n_1\varepsilon_1 + n_2\varepsilon_2 + \cdots + n_d\varepsilon_d \mid n_1, n_2, \ldots, n_d \in \mathbb{Z}\} = \{\mathbf{n}\cdot\boldsymbol{\varepsilon} \mid \mathbf{n} \in \mathbb{Z}^d\}, \quad (2.22)$$

where $\{\varepsilon_j\}$ are the primitive vectors of the lattice. For our purposes, we can identify $\mathbf{n}\cdot\boldsymbol{\varepsilon}$ with $\mathbf{n}$.

Fermions on the lattice are described by smeared out creation and annihilation operators $c^\dagger$ and c satisfying the canonical anticommutation relations. The smearing is by square summable sequences on the lattice:

$$\ell^2(\mathbb{Z}^d) \ni \varphi \mapsto c^\dagger(\varphi) \text{ is } \mathbb{C}\text{-linear} \quad (2.23)$$

and the anticommutation relations are

$$\{c(\varphi), c(\psi)\} = 0 \text{ and } \{c(\varphi), c^\dagger(\psi)\} = \langle\varphi,\psi\rangle\mathbb{1}. \quad (2.24)$$

The creation and annihilation operators generate the C*-algebra $\mathcal{A}(\mathbb{Z}^d)$ of canonical anticommutation relations on $\mathbb{Z}^d$ (CAR).

Lattice translations induce $*$-automorphisms on $\mathcal{A}(\mathbb{Z}^d)$ by extending

$$c(\varphi) \mapsto c(U(\mathbf{n})\varphi). \quad (2.25)$$

Here $U(\mathbf{n})$ is the unitary shift on $\ell^2(\mathbb{Z}^d)$ by $\mathbf{n} \in \mathbb{Z}^d$

$$\big(U(\mathbf{n})\,\varphi\big)(\mathbf{k}) = \varphi(\mathbf{k}-\mathbf{n}). \quad (2.26)$$

We also need quasi-free states ω_Q, sometimes called Gaussian Fermionic states. They are uniquely determined by their two-point correlation functions

$$(\varphi,\psi) \mapsto \omega\big(c^\dagger(\varphi)c(\psi)\big), \quad \varphi,\psi \in \ell^2(\mathbb{Z}^d). \quad (2.27)$$

All expectations of monomials in creation and annihilation operators vanish except for

$$\omega\big(c^\dagger(\varphi_1)\cdots c^\dagger(\varphi_n)c(\psi_n)\cdots c(\psi_1)\big) = \det\Big(\big[\omega\big(c^\dagger(\varphi_k)c(\psi_\ell)\big)\big]_{k\ell}\Big). \quad (2.28)$$

Due to the complex linearity of $c^\dagger$, and the conjugate linearity of c,

$$(\varphi, \psi) \mapsto \omega\big(c^\dagger(\varphi)c(\psi)\big) \tag{2.29}$$

is a sesquilinear form on $\ell^2(\mathbb{Z}^d)$. One can show that the necessary and sufficient condition for (2.28) to define a state is that the form (2.29) corresponds to a linear operator Q on $\ell^2(\mathbb{Z}^d)$ such that $0 \leq Q \leq \mathbb{1}$:

$$\omega\big(c^\dagger(\varphi)c(\psi)\big) = \langle \psi, Q\,\varphi\rangle. \tag{2.30}$$

The operator Q, called the symbol, defines the state ω_Q, where the notation stresses the dependence of the state ω on Q.

A quasi-free state ω_Q is shift-invariant if and only if Q commutes with the lattice-shift unitaries $U(\mathbf{n})$ defined in (2.26). In the standard basis $\{e_\mathbf{j}\}$ of $\ell^2(\mathbb{Z}^d)$ this is equivalent with

$$\langle e_\mathbf{j}, Q\, e_\mathbf{k}\rangle = \langle e_{\mathbf{j}+\mathbf{n}}, Q\, e_{\mathbf{k}+\mathbf{n}}\rangle, \;\; \mathbf{j}, \mathbf{k}, \mathbf{n} \in \mathbb{Z}^d. \tag{2.31}$$

If F denotes the unitary Fourier transformation

$$(F\,\varphi)(\mathbf{x}) := \sum_{\mathbf{n}\in\mathbb{Z}^d} \varphi(\mathbf{n})\, \mathrm{e}^{2\pi i \mathbf{n}\cdot\mathbf{x}}, \;\; \mathbf{x} \in [0,1]^d \tag{2.32}$$

this is equivalent to

$$F\,Q\,F^\dagger = q \tag{2.33}$$

where q is the multiplication operator with the function

$$q(\mathbf{x}) = \sum_{\mathbf{j}\in\mathbb{Z}^d} \langle e_\mathbf{0}, Q\, e_\mathbf{j}\rangle\, \mathrm{e}^{2\pi i \mathbf{j}\cdot\mathbf{x}} \tag{2.34}$$

on $\mathcal{L}^2([0,1]^d)$. As $0 \leq Q \leq \mathbb{1}$, q_x takes values in $[0,1]$. For more details on these matters we refer to [12, 20, 22].

2.4 Rényi entropies

Let Λ be a finite subset of $\mathbb{Z}^d$. The local algebra $\mathcal{A}(\Lambda)$ is generated by the creation and annihilation operators with smearing functions supported in Λ. This algebra is isomorphic to the algebra of matrices of dimension $2^{\#(\Lambda)}$ and has therefore, up to unitary equivalence, a unique irreducible representation. This allows one to assign to any state ω on $\mathcal{A}(\Lambda)$ the Rényi entropies

$$\mathsf{S}_\alpha(\omega) := -\frac{1}{\alpha - 1} \log \mathrm{Tr}\, \rho^\alpha, \;\; \alpha > 0. \tag{2.35}$$

Here ρ is the density matrix defining ω in an irreducible representation of $\mathcal{A}(\Lambda)$. For $\alpha = 1$, the expression in (2.35) has to be replaced by its limit, the von Neumann entropy

$$\mathsf{S}_\alpha(\omega) := \mathsf{S}_1(\omega) = -\mathrm{Tr}\,(\rho \log \rho). \tag{2.36}$$

The local Rényi entropies of quasi-free states can be readily expressed in terms of the local restrictions of their corresponding symbols Q. Moreover, one can show that for shift-invariant quasi-free states the limiting average Rényi entropies in the sense of growing boxes exist and one obtains an explicit expression in terms of the Fourier transform q_x:

$$\mathsf{s}_q(\alpha) = -\frac{1}{\alpha - 1} \int_{[0,1]^d} d\mathbf{x}\, \log\big(q(\mathbf{x})^\alpha + (1 - q(\mathbf{x}))^\alpha\big). \tag{2.37}$$

One may remark that the above form is quite natural. One can easily see that in the case of a shift-invariant pure state, where $q(\mathbf{x}) = 0$ or $q(\mathbf{x}) = 1$, the average entropy is zero.

In the case of the von Neumann entropy density, this expression must again be understood as

$$\mathsf{s}_q = -\int_{[0,1]^d} d\mathbf{x}\, \big[q(\mathbf{x}) \log q(\mathbf{x}) + (1 - q(\mathbf{x})) \log(1 - q(\mathbf{x}))\big]. \tag{2.38}$$

2.5 A completely monotonic entropy

It is known that for a general density matrix ρ in a matrix algebra

$$\alpha \in]0, \infty[\mapsto -\frac{1}{\alpha - 1}\, \log \mathrm{Tr}\, \rho^\alpha \tag{2.39}$$

is a monotonically decreasing function [5], in particular

$$\mathsf{S}_\rho \geq \mathsf{S}_\rho(2) \geq \mathsf{S}_\rho(3) \geq \cdots \tag{2.40}$$

This ordering then extends to densities, provided they exist. This is certainly the case for shift-invariant quasi-free states, where it is not hard to compute the asymptotic value

$$\mathsf{s}_q(\infty) = \lim_{\alpha \to \infty} \mathsf{s}_q(\alpha) = -\int_{[0,1]^d} d\mathbf{x}\, \log\big[\max\{q(\mathbf{x}), (1 - q(\mathbf{x}))\}\big]. \tag{2.41}$$

For a more detailed treatment of what is currently known about Rényi entropies in the context of quantum systems, the reader may refer to [47].

We now introduce a modified entropy-like function:

$$g_q(\alpha) := \mathsf{s}_q(\infty) - \tfrac{\alpha-1}{\alpha}\,\mathsf{s}_q(\alpha), \;\; \alpha > 0. \tag{2.42}$$

The motivation for reforming the entropy in this way may seem unclear now, but the reasoning will be made clear later on. To avoid technical complications, we assume from now on that $q(\mathbf{x}) = 0$ or $q(\mathbf{x}) = 1$ on a set of measure zero. The general case can be handled by removing the union of the kernels of $q(\mathbf{x})$ and $1 - q(\mathbf{x})$ from $[0,1]^d$. One now easily verifies that

$$g_q(\alpha) = \frac{1}{\alpha}\int_{[0,1]^d} d\mathbf{x}\, \log[1 + \exp(-\alpha h)], \tag{2.43}$$

where we have introduced the function

$$h(\mathbf{x}) : [0,1]^d \to \mathbb{R}^+ : \mathbf{x} \to h(\mathbf{x}) := -\log\Big(\min\Big\{\frac{q(\mathbf{x})}{1-q(\mathbf{x})}, \frac{1-q(\mathbf{x})}{q(\mathbf{x})}\Big\}\Big). \tag{2.44}$$

A function $f :]0,\infty[\to \mathbb{R}$ is called completely monotonic if its derivatives to all orders exist and if

$$(-1)^n f^{(n)} \geq 0, \;\; n = 0, 1, 2, \ldots \tag{2.45}$$

Bernstein's theorem [8, 44] characterises completely monotonic functions as the Laplace transforms of positive measures that don't grow too fast at infinity. A useful review of monotonic functions and their properties can be found in [35].

We show here that, for a given q_x,

$$\alpha \in]0,\infty[\mapsto g_q(\alpha) \tag{2.46}$$

is completely monotonic by computing its inverse Laplace transform.

First, consider the function k on $\mathbb{R}^+$:

$$k(t) = \sum_{\substack{j\in\mathbb{N}_0 \\ j\leq t}} \frac{(-1)^{j+1}}{j}, \;\; t \geq 0. \tag{2.47}$$

This function is piecewise constant, non-negative, continuous from the right, and tends to $\log 2$, see Fig. 2.4.

Definition 1 (Exponential order)**.** Given the function $f(t)$ and real, strictly positive constants C, t_0 and a satisfying the constraint $\forall t \geq t_0 : |f(t)| < Ce^{at}$, $f(t)$ is said to be of exponential order equal to $\inf a$, the infimum over all a satisfying the constraint.

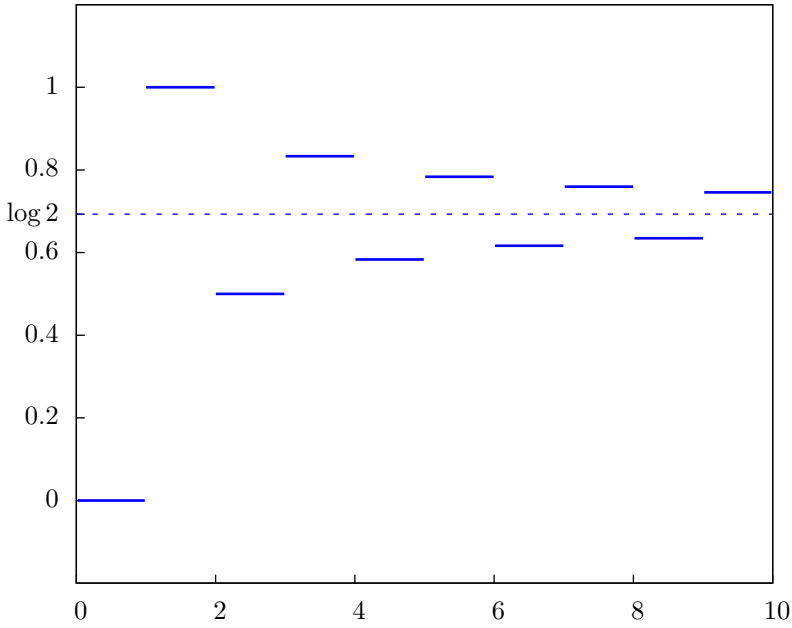

Figure 2.4: The inverse Laplace transform of $s \mapsto \log(1+\exp(-s))/s$

As k is of exponential order 0, meaning that it does not grow 'too quickly' and so the Laplace transform exists, we may compute its Laplace transform for all $s \in \mathbb{C}$ with $\Re(s) > 0$ by evaluating the integral

$$\begin{aligned}\mathcal{L}(k)(s) &= \int_{\mathbb{R}^+} dt\, k(t)\, \mathrm{e}^{-st} = \sum_{\ell=1}^{\infty} \sum_{j=1}^{\ell} \frac{(-1)^{j+1}}{j} \int_{\ell}^{\ell+1} dt\, \mathrm{e}^{-st} \\ &= \sum_{\ell=1}^{\infty} \frac{1}{s} \left(\mathrm{e}^{-\ell s} - \mathrm{e}^{-(\ell+1)s}\right) \Big(\sum_{j=1}^{\ell} \frac{(-1)^{j+1}}{j}\Big) \\ &= \frac{1}{s} \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+1}}{\ell}\, \mathrm{e}^{-\ell s} = \frac{1}{s}\, \log\big(1+\exp(-s)\big). \end{aligned} \tag{2.48}$$

This shows that

$$s > 0 \mapsto \frac{1}{s}\, \log\big(1+\exp(-s)\big) \tag{2.49}$$

is completely monotonic.

As complete monotonicity is preserved by rescaling the argument, rescaling the function, and addition, we conclude from (2.43) that

$$\alpha \in]0,\infty[\mapsto g_{q_x}(\alpha) \tag{2.50}$$

is completely monotonic. We have, in fact, a rather explicit expression for the inverse Laplace transform of g_{q_x}:

$$\mathcal{L}^{-1}\big(g_{q_x}\big)(t) = \int_{[0,1]^d} d\mathbf{x}\, k\Big(\frac{t}{h}\Big). \tag{2.51}$$

2.6 Reconstructing the von Neumann entropy

In general, one cannot hope to uniquely reconstruct a function g that is analytic in $\{z \in \mathbb{C} \mid \Re(z) > 0\}$ given the values of g on $\mathbb{N}_0$. This is nevertheless often attempted in statistical mechanics of disordered systems where one tries to reconstruct the von Neumann entropy given the Rényi entropies of order 2, 3, ... which can be computed using the replica trick. Suppose, however, that there exists a non-negative measurable function G of exponential order 0 on $\mathbb{R}^+$ such that

$$g_q(\alpha) = \int_0^\infty dt\, G(t,q)\, \mathrm{e}^{-\alpha t}, \;\; \alpha > 0 \tag{2.52}$$

where g_q is related to the average entropies s as in (2.42). We then have

$$\mathsf{s}_q(\alpha) = \frac{\alpha}{\alpha - 1} \int_0^\infty dt\, G(t,q) \left(\mathrm{e}^{-t} - \mathrm{e}^{-\alpha t}\right), \;\; \alpha \neq 1 \tag{2.53}$$

and

$$\mathsf{s}_q = \mathsf{s}_q(1) = \int_0^\infty dt\, G(t,q)\, t\, \mathrm{e}^{-t}. \tag{2.54}$$

Suppose that we know the integer-order average entropy $\mathsf{s}(n)$ for $n = 2, 3, \ldots$ and that we wish to reconstruct the average von Neumann entropy$\mathsf{s}$ given (2.53) and (2.54). The vector space generated by the functions

$$f_n : t \in \mathbb{R}^+ \mapsto \frac{n}{n-1} \left(\mathrm{e}^{-t} - \mathrm{e}^{-nt}\right), \;\; n = 2, 3, \ldots \tag{2.55}$$

is actually an algebra of continuous functions that vanish at 0 and at ∞. It is closed under complex conjugation and it separates the points in $\mathbb{R}^+$. We can therefore approximate

$$t \in \mathbb{R}^+ \mapsto t\, \mathrm{e}^{-t} \tag{2.56}$$

uniformly to arbitrary precision by a linear combination of the f_n using the Stone-Weierstrass theorem [11]. It should become clear now, that the reason for choosing a representation of the average Rényi entropy in Fourier space, is to be able to recast it in an exponential form compatible with the use of the Stone-Weierstrass theorem, which states that every continuous function defined on a closed interval can be uniformly approximated as closely as desired by a polynomial function.

Theorem 2. *Let $C(X)$ be the ring of continuous functions on a compactum X with the topology of uniform convergence, i.e. the topology generated by the norm*

$$\|f\| = \max_{x\in X} |f(x)|\,, \quad f \in C(X),$$

and let $C_0 \subseteq C(X)$ be a subring containing all constants and separating the points of X, i.e. for any two different points $x_1, x_2 \in X$ there exists a function $f \in C_0$ for which $f(x_1) \neq f(x_2)$. Then $[C_0] = C(X)$, i.e. every continuous function on X is the limit of a uniformly converging sequence of functions in C_0.

Given a d-dimensional density matrix ρ and $d-1$ Rényi entropies of integer order in $\{2, 3, \ldots\}$ we can uniquely reconstruct the ordered eigenvalues of ρ. This means that two density matrices with the same integer Rényi entropies are related by a unitary transformation.

The average Rényi entropies of a shift-invariant quasi-free state are of the form $\int_{[0,1]^d} d\mathbf{x}\, f(q(\mathbf{x}))$ where f is a bounded measurable function on $[0,1]$. We can associate a distribution function to a symbol $q(\mathbf{x})$ in Fourier space as follows,

$$\gamma_q : y \in [0,1] \mapsto \int_{\substack{[0,1]^d \\ q(\mathbf{x})\leq y}} d\mathbf{x}. \tag{2.57}$$

We can then write

$$\int_{[0,1]^d} d\mathbf{x}\, f(q(\mathbf{x})) = \int_0^1 d\gamma_q(y)\, f(y). \tag{2.58}$$

Obviously, different symbols may yield the same distribution function and therefore the same average Rényi entropies. Knowledge of the integer average entropies with $\alpha \in \{2, 3, \ldots\}$ actually determines the distribution function except for contributions at 0 or 1 which don't effectively contribute to any average entropy for $\alpha > 0$.

Suppose that t is a Lebesgue measure preserving rearrangement of $[0,1]^d$, i.e. a transformation of $[0,1]^d$ such that

$$\int_{\mathbf{x}\in\Lambda} d\mathbf{x} = \int_{t(\mathbf{x})\in\Lambda} d\mathbf{x} \tag{2.59}$$

for every measurable set Λ. The mapping

$$U_t : \varphi \mapsto \varphi \circ t \tag{2.60}$$

is a unitary transformation of $\mathcal{L}^2([0,1]^d)$ such that for a multiplication operator by q

$$U_t\, q = (q \circ t)\, U_t. \tag{2.61}$$

The Fourier transformed symbols q and $q \circ t$ define different shift-invariant quasi-free states on $\mathcal{A}(\mathbb{Z}^d)$ which are related by the automorphism defined through U_t.

The distribution functions (2.57) of these states coincide and therefore have the same average entropies. This situation can be seen as a partial quasi-free analogue of the density matrix case discussed above. There are, however, plenty of symbols that yield the same average entropies and that are not related by a rearrangement.

2.7 Explicit approximations

Let us extend the notation in (2.55) by defining

$$f_1(t) = t\mathrm{e}^{-t}. \tag{2.62}$$

A simple proposal for an n-term approximation of f_1 consists in finding the minimisers of

$$(\gamma_1, \ldots, \gamma_n) \mapsto \|f_1 - \gamma_1\, f_2 - \cdots - \gamma_n\, f_{n+1}\|_\infty \tag{2.63}$$

by demanding that all extrema of the above function are equal in magnitude. The first few optimal approximations are

$$\begin{aligned}
&\|f_1 - 0.800\, f_2\|_\infty = 0.09\\
&\|f_1 - 2.219\, f_2 + 1.314\, f_3\|_\infty = 0.04\\
&\|f_1 - 4.233\, f_2 + 6.133\, f_3 - 2.850\, f_4\|_\infty = 0.02\\
&\|f_1 - 6.833\, f_2 + 17.498\, f_3 - 18.780\, f_4 + 7.148\, f_5\|_\infty = 0.01.
\end{aligned} \tag{2.64}$$

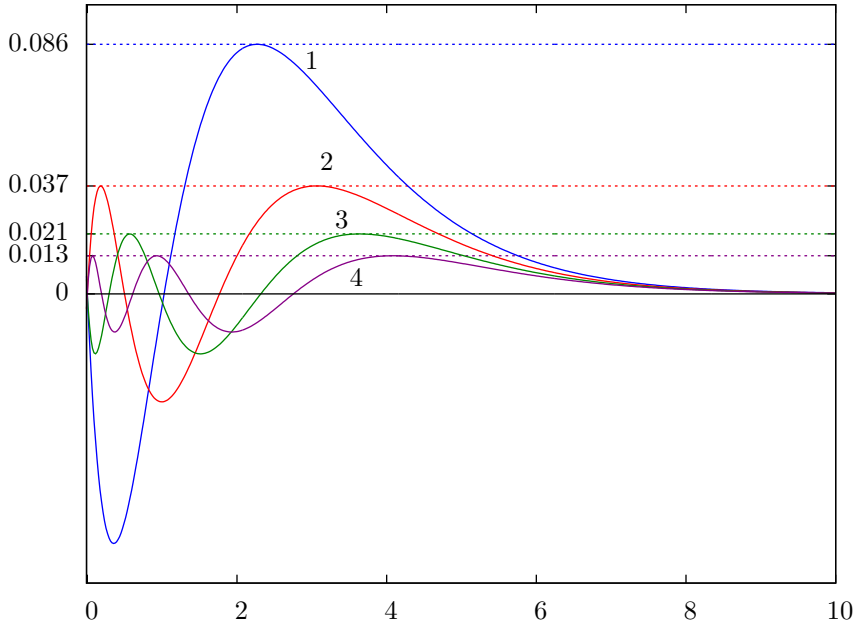

Figure 2.5: Difference between te^{-t} and its 1, 2, 3 and 4-term approximations as indicated, given by Equation (2.63)

In comparison, $\|f_1\|_\infty \approx 0.368$. The approximation technique is based on an optimisation; for any particular choice of approximation terms, their corresponding coefficients are chosen in such a way that all the extrema of the resulting function (the approximation's largest deviation from the target function) are equalised. When all extrema are equal in magnitude, this corresponds to the best possible choice of the coefficients. This can be seen in Figure (2.5), where the maxima and minima for each approximation are equal in magnitude.

This corresponds to the approximations of the average von Neumann entropy by the first few average Rényi entropies

$$\begin{aligned}
\mathsf{s}_q &\approx 0.800\,\mathsf{s}_q(2)\\
&\approx 2.219\,\mathsf{s}_q(2) - 1.314\,\mathsf{s}_q(3)\\
&\approx 4.233\,\mathsf{s}_q(2) - 6.133\,\mathsf{s}_q(3) + 2.850\,\mathsf{s}_q(4)\\
&\approx 6.833\,\mathsf{s}_q(2) - 17.498\,\mathsf{s}_q(3) + 18.780\,\mathsf{s}_q(4) - 7.148\,\mathsf{s}_q(5)
\end{aligned} \tag{2.65}$$

The single term approximation is certainly terrible because we already know from the monotonicity of the Rényi entropy densities that

$$\mathsf{s}_q \geq \mathsf{s}_q(2). \tag{2.66}$$

The multi-term approximations are, however, no longer direct consequences of the monotonicity of the Rényi densities. The quality of (2.65) is not easily assessed because the measure $G(t,q)dt$ is generally unbounded.

Under our assumption on $q(\mathbf{x})$, the function G in (2.53) tends to $\log 2$ at infinity. As the supremum norm is attained close to the origin, we cannot expect to obtain a very good approximation this way. A better approach, especially at high temperatures, is to subtract the asymptotic value $\log 2$ from G and then use (2.64). This yields

$$\begin{aligned}
\mathsf{s}_q &\approx 0.200\,\log 2 + 0.800\,\mathsf{s}_q(2)\\
&\approx 0.095\,\log 2 + 2.192\,\mathsf{s}_q(2) - 1.314\,\mathsf{s}_q(3)\\
&\approx 0.050\,\log 2 + 4.233\,\mathsf{s}_q(2) - 6.133\,\mathsf{s}_q(3) + 2.850\,\mathsf{s}_q(4)\\
&\approx 0.033\,\log 2 + 6.833\,\mathsf{s}_q(2) - 17.498\,\mathsf{s}_q(3) + 18.785\,\mathsf{s}_q(4) - 7.148\,\mathsf{s}_q(5)
\end{aligned} \tag{2.67}$$

One can, however, still not hope that $G - \log 2$ is integrable.

A controllable approximation scheme can be set up by using Rényi densities of order less than one and using the uniform bound

$$\mathsf{s}_q(\alpha) = \frac{\alpha}{\alpha - 1} \int_0^\infty dt\, G(t, q_x) \left(\mathrm{e}^{-t} - \mathrm{e}^{-\alpha t}\right) \leq \log 2. \tag{2.68}$$

Extending the definition of f_n in (2.55) to general $\alpha \in \mathbb{R}^+$ we write

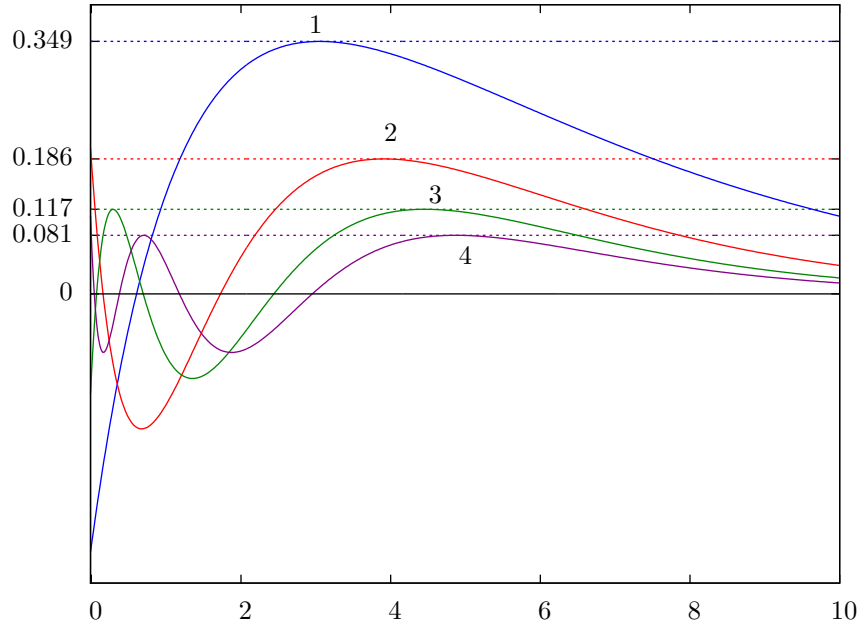

Figure 2.6: Difference between f_1/f_α and its controlled 1, 2, 3 and 4-term approximations re-scaled by f_α, given by Equations (2.69)

$$
\begin{aligned}
&\Big|\mathsf{s}_q - \gamma_1\,\mathsf{s}_q(2) - \cdots - \gamma_n\,\mathsf{s}_q(n+1)\Big| \\
&\quad = \Big|\int_0^\infty dt\,G(t,q_x)\,\Big(f_1(t) - \gamma_1\,f_2(t) - \cdots - \gamma_n\,f_{n+1}(t)\Big)\Big| \\
&\quad = \Big|\int_0^\infty dt\,G(t,q_x)\,f_\alpha(t)\,\Big(\frac{f_1(t)}{f_\alpha(t)} - \gamma_1\,\frac{f_2(t)}{f_\alpha(t)} - \cdots - \gamma_n\,\frac{f_{n+1}(t)}{f_\alpha(t)}\Big)\Big| \\
&\quad \leq \Big\|\frac{f_1}{f_\alpha} - \gamma_1\,\frac{f_2}{f_\alpha} - \cdots - \gamma_n\,\frac{f_{n+1}}{f_\alpha}\Big\|_\infty\,\log 2. \qquad (2.69)
\end{aligned}
$$

It now remains to minimise the bound (2.69) for a given n with respect to $\gamma_1, \ldots, \gamma_n$ and $\alpha \in]0, 1[$. This leads to

$$\begin{aligned}
&\left|\mathsf{s}_q - 0.666\,\mathsf{s}_q(2)\right| \leq 0.35\\
&\left|\mathsf{s}_q - 1.938\,\mathsf{s}_q(2) + 1.005\,\mathsf{s}_q(3)\right| \leq 0.19\\
&\left|\mathsf{s}_q - 3.892\,\mathsf{s}_q(2) + 4.967\,\mathsf{s}_q(3) - 2.048\,\mathsf{s}_q(4)\right| \leq 0.12\\
&\left|\mathsf{s}_q - 6.556\,\mathsf{s}_q(2) + 15.064\,\mathsf{s}_q(3) - 14.413\,\mathsf{s}_q(4) + 4.923\,\mathsf{s}_q(5)\right| \leq 0.08\\
&\ldots\\
&\Big|\mathsf{s}_q - 37.181\,\mathsf{s}_q(2) + 529.415\,\mathsf{s}_q(3) - 3\,846.261\,\mathsf{s}_q(4) + 16\,301.725\,\mathsf{s}_q(5)\\
&\quad - 43\,168.833\,\mathsf{s}_q(6) + 73\,647.855\,\mathsf{s}_q(7) - 80\,999.681\,\mathsf{s}_q(8) + 55\,517.489\,\mathsf{s}_q(9)\\
&\quad - 21\,580.373\,\mathsf{s}_q(10) + 3\,634.848\,\mathsf{s}_q(11)\Big| \leq 0.03
\end{aligned} \tag{2.70}$$

The corresponding values for α are: 0.661, 0.515, 0.435, 0.384, and 0.261 respectively. As before, the coefficients are optimally chosen in such a way that all extrema of the resulting function are equal in magnitude, as shown in Figure (2.6). The improvement in this case comes from the added freedom that the value of the function at zero is no longer fixed at zero but is included in the set of extrema which should be equal in magnitude. Contrasted with Figure (2.5), one can see the effect of the added degree of freedom in allowing the function to take a non-zero value for a zero abscissa.

2.8 Conclusion

In this chapter, we considered the reconstruction of the average von Neumann entropy in terms of average Rényi entropies of integer order which, for some classes of states, can be very easily computed. Obtaining general estimates of and relations between these quantities has been a long-standing problem.

The early sections of the chapter explore naive attempts at a direct reconstruction, first of the density matrix and then of the transition matrix. Both of these are highly nonlinear. Since we are interested in entropy densities in the thermodynamic limit, the former is not useful and the latter does not lead to non-trivial bounds in the limit.

The example given in Section (2.2) introduces the idea of a linear reconstruction in the very simple case of a chain in a product state. While the idea is certainly in the spirit of what we would like to achieve, the choice of orders of the Rényi entropes used to construct the approximation is not easy to optimise and we do not wish to limit ourselves to product states.

Instead, we have restricted our attention to shift-invariant quasi-free Fermionic states on a regular lattice and obtained two results. Firstly, we proved that the average von Neumann entropy is reconstructible in terms of average Rényi entropies of integer order.

Next, we set up an explicit approximation scheme. This scheme, including the controlled approximations (2.70), relies only on the validity of the representation (2.53) and is therefore applicable to general systems for which (2.53) holds and is not only limited to the shift-invariant quasi-free states considered here. Of course, the $\log 2$ asymptotic limit given in the controlled approximation scheme should be adjusted according to the dimensionality of the states in question. It should be noted that the coefficients in (2.64) and (2.70) are not easily expressible in a general analytical form. Moreover, the obtained approximations are generally neither upper nor lower bounds.

Chapter 3

Modelling dynamics

The previous chapter dealt with entropies of states. In this chapter we try to explore similar concepts for dynamical systems; in other words, a system which evolves in time according to some prescribed rules. These rules are generally prescribed by the system's Hamiltonian, which may or may not be time independent, which invariably leads to unitary reversible dynamics.

If one considers a closed system evolving autonomously and wishes to describe the state of some subsystem thereof, this can be done by "averaging out" (formally, by taking a partial trace) over the degrees of freedom in which one is not interested. This averaging out through the partial trace is irreversible. This is because the act of averaging out results in a loss of information about the original state, and so there is generally no unique way to expand the reduced system back into the full space again. As a consequence, the dynamics of the reduced system are such that future dynamics depend strongly on its history and a general description of such dynamics is a very hard problem.

In general, the total system including the environment exists as a pure state and the reduced system's state after tracing out the environment is a mixed state. Despite this loss of information about the environment after a partial trace, it is still possible to say something about the behaviour of the reduced system if some very strong assumptions are made on the environment and how it interacts with the reduced system; these assumptions will be discussed in more detail later.

If one considers the dynamics of this reduced system, referred to as the reduced dynamics, it will certainly not be unitary or reversible, but under certain strong assumptions it can still be thought of in terms of a "black box" which takes

the initial reduced system's state as an input state and gives the time-evolved reduced system's state as an output.

Each use of this black-box can be thought of as a discrete step forward in time, iterating over many uses can generate the reduced system's state any number of discrete time-steps in the future.

Such black-box dynamics typically result in a change in entropy between the input and output states. Questions one could ask about such dynamics include "Does the system have some equilibrium state under these dynamics and if so, what is it?" or "What is the maximum entropy difference between input and output states?"

If these aforementioned strong assumptions are met and we are able to construct a dynamical process in the form of a black-box dynamics which maps the state of a reduced system at some arbitrary initial time to an evolved state at some later time, then we may notice that, on average, with each successive use of the black-box we lose a little bit of information on the initial conditions.

This loss of information comes about due to the interaction with and eventual averaging out over the environmental degrees of freedom and typically results in a gain of entropy in the reduced system. The rate at which this information is lost, or the rate at which entropy is produced by this process, is termed the dynamical entropy, the entropy density, the average entropy or the entropy production rate of the process.

This chapter presents one particular black-box model and explores questions related to dynamical entropies. This is done through an artificial model of a process, built up using a combination of some prescribed black-box dynamics and a certain type of generalised measurement which shall be introduced in detail later. By periodically probing the system with a series of these generalised measurements at discrete times, between which leaving it to evolve autonomously according to the black-box dynamics, we can build up a chain of correlations. Moving right one space on this discrete chain is equivalent to moving one time-step forwards.

The results of the generalised measurements after n time-steps is encoded into the nth site on the chain. In this way, a detailed model of the time-evolution of a system is constructed which contains all multi-time correlation-functions, and it is the entropic characteristics of this model which is the focus of the following two chapters.

3.1 Deterministic dynamics of quantum systems

3.1.1 Closed quantum systems

The rules governing the time evolution of the state of a finite closed system are defined by the system's Hamiltonian $H(t)$, a Hermitian operator corresponding to the total energy of the system. The Hamiltonian generates a system's dynamics through the time-dependent Schrödinger equation,

$$\frac{d}{dt}|\Psi(t)\rangle = -\frac{\imath}{\hbar}H(t)|\Psi(t)\rangle. \tag{3.1}$$

A solution to this differential equation may be written as

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle, \tag{3.2}$$

for some initial state $|\Psi(t_0)\rangle$ at initial time $t = t_0$ where $U(t_0,t_0) = \mathbb{1}$. $U(t,t_0)$ is a unitary operator, referred to as the time-evolution operator, which also satisfies the Schrödinger equation,

$$\frac{d}{dt}U(t) = -\frac{\imath}{\hbar}H(t)U(t). \tag{3.3}$$

The unitarity of U is ensured by the Hermiticity of the Hamiltonian H, and it is the Hamiltonian that generates the time-evolution through equation (3.3) and fully determines everything connected with a closed system's time evolution.

If the Hamiltonian is not time-dependent, i.e., an autonomous system where $H(t) = H$, then

$$U(t,t_0) = U(t-t_0) = \exp\left(-\imath(t-t_0)H/\hbar\right). \tag{3.4}$$

If the Hamiltonian depends on time, then we cannot express $U(t,t_0)$ in closed form but instead in terms of a time-ordered exponential,

$$U(t,t_0) = T_{\leftarrow}\exp\frac{\imath}{\hbar}\int_{t_0}^{t} H(s)ds, \tag{3.5}$$

where $T_{\leftarrow}$ represents the chronological time-ordering operator which orders products of time-dependent operators such that their arguments increase from right to left.

In either case, the evolution in time of an isolated quantum system is unitary. This unitary evolution preserves the inner product of a state bra with another state ket,

$$\langle\psi|\phi\rangle \to \langle\psi|U^\dagger U|\phi\rangle = \langle\psi|\phi\rangle, \tag{3.6}$$

and the commutation relations between observables are invariant under the dynamics.

As a consequence of multiplicative associativity, there is a mathematical duality between considering the expectation of some observable X in some time-evolved state $U|\phi\rangle$ and some time-evolved observable $U^\dagger XU$ in some state $|\phi\rangle$,

$$\langle\psi|\phi\rangle \to \left(\langle\psi|U^\dagger\right) X \left(U|\phi\rangle\right) = \langle\psi| \left(U^\dagger XU\right) |\phi\rangle. \tag{3.7}$$

This duality highlights two equivalent approaches. In the first, the Schrödinger picture, states are seen to evolve in time and observables do not. In the second, the Heisenberg picture, the observables evolve in time and the states do not.

The time-evolution of a density operator whose initial state at time $t = t_0$ is $\rho(t_0)$ can be expressed as

$$\rho(t) = U(t - t_0)\rho(t_0)U^\dagger(t - t_0). \tag{3.8}$$

The spectrum of any density operator is invariant under any unitary transform, including the time-evolution operator. We can write the equation of motion for a density operator as

$$\frac{d\rho(t)}{dt} = \frac{-\imath}{\hbar} \left[H(t), \rho(t)\right]. \tag{3.9}$$

The autonomous evolution of finite, closed quantum systems is unitary, fully deterministic and divisible. Divisibility, in the sense that one may divide the trajectory into arbitrarily fine time-slices, is a consequence of autonomous Hamiltonian dynamics and is generally not a property enjoyed by open systems. Because of the unitarity and divisibility of the dynamics, the entropy of quantum states under such dynamics is preserved and knowing the state of the system at any one time is sufficient to calculate the state at any point in its future.

3.1.2 Open quantum systems

While an isolated quantum system undergoes unitary evolution, the evolution of a system which is connected to some environment (an open system) is somewhat

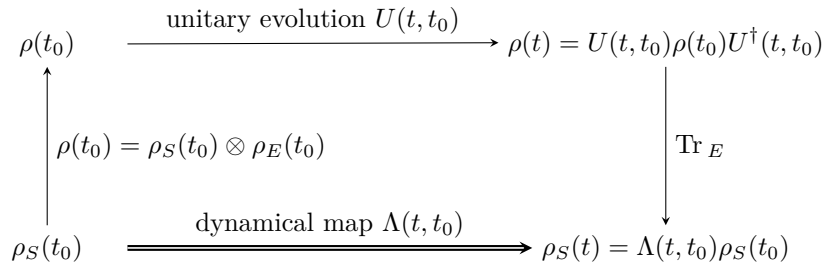

Figure 3.1: Commutative diagram showing the connection between unitary evolution, tracing out the environment and the dynamical map $\Lambda(t, t_0)$.

more complicated. In general, the evolution of open quantum systems need not be unitary. Additional complications arise in that the time-evolution of an open quantum system is generally not divisible and in order to determine the state at some point in the future one requires detailed knowledge of the system's history; these dependencies are usually referred to as memory effects.

One can think of an open quantum system in terms of some system of interest, whose state is given in terms of the density matrix ρ_S living in $\mathcal{H}_S$, which is connected to some environment, whose state is given in terms of the density matrix ρ_E living in $\mathcal{H}_E$. Together, the total system with density matrix ρ, living in the composite space $\mathcal{H}_S \otimes \mathcal{H}_E$, still evolves unitarily, as described previously.

The dynamics of the subsystem ρ_S induced by the Hamiltonian evolution of the total system is referred to as the reduced dynamics, which can always be found by tracing out the environmental degrees of freedom leaving us with the reduced system,

$$\rho_S(t) = \mathrm{Tr}_E \left\{ U(t,t_0)\rho(t_0)U^\dagger(t,t_0) \right\}. \tag{3.10}$$

Since this trace over the environment is irreversible, i.e., there exists no unique composite state which corresponds to a given reduced state, the reduced dynamics can only be determined if one fully specifies the total composite state at the initial time. This is usually taken to be a product state,

$$\rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0). \tag{3.11}$$

In many situations, it is useful to describe the dynamics of an open quantum system by formulating appropriate equations of motion for its density matrix, known as a quantum master equation. In general, such dynamics of reduced systems are quite complicated. If we consider only environments with short

correlation-times, we would be justified in neglecting memory effects and describing the reduced dynamics in terms of a one-parameter quantum dynamical semigroup. Such dynamics are called "memoryless" because all future states are fully determined with only the information of the current state; past states have no bearing on future dynamics.

It is therefore necessary to make some assumptions/approximations.

- Born approximation

  The interaction between the system and the environment is very weak compared with their self-interactions.

- Markov approximation

  The correlation times of the environment are much shorter than the time-scales of the system dynamics. This has the consequence that the dynamics are memoryless.

- Initial state

  The initial state of the total system is assumed to be a product state, as in Equation (3.11). In other words, the system and environment are initially uncorrelated at time $t = t_0$.

The reduced dynamics can then be characterised by means of a dynamical map [17, 31], mapping density matrices to density matrices, in terms of $\mathcal{H}_S$ only:

$$\Lambda(t, t_0) : \mathcal{S}(\mathcal{H}_S) \mapsto \mathcal{S}(\mathcal{H}_S), \tag{3.12}$$

so that $\rho_S(t) = \Lambda(t, t_0)\rho_S(t_0)$. The relationships between the full and reduced systems both at some initial time $t = t_0$ and after evolving until some later time t is depicted in Figure (3.1).

Henceforth, only autonomous evolution will be considered; this results in a simplified picture where the unitary time-evolution operator $U(t, t_0)$ has the groupoid property $U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0)$. We can then express the time-evolution operator as $U(t - t_0)$ because it is only the time difference which is relevant. As a consequence of this divisibility on the level of the Hamiltonian dynamics and the assumptions/approximations outlined earlier, the dynamical map Λ also enjoys this property, also referred to as the Markov or semigroup property, and can be expressed in terms of a time difference as $\Lambda(t - t_0)$.

Considering this map $\Lambda(t - t_0)$, we can allow t to vary resulting in a one-parameter family of dynamical maps $\{\Lambda(t - t_0) : t \geq t_0\}$ where $\Lambda(0) = \mathrm{id}$ is just the identity operator.

If one starts from the assumption of an initial product state as in Equation (3.11) and that the environment is initially in its (pure) ground state $|0\rangle$, one can then explicitly calculate the partial trace in Equation (3.10), arriving at

$$\rho(t) = \Lambda(t - t_0)\rho_S(t_0) = \sum_i K_i(t - t_0)\rho_S(t_0)K_i^\dagger(t - t_0), \tag{3.13}$$

where

$$K_i(t - t_0) = \langle e_i|U(t - t_0|0\rangle). \tag{3.14}$$

The operators K_i are called Kraus operators and satisfy

$$\sum_i K_i K_i^\dagger = \mathbb{1} \tag{3.15}$$

if and only if they correspond to a completely-positive trace-preserving map [31]. The notion of complete positivity will be defined shortly.

The Kossakowski–Lindblad equation is considered to be the most general Markovian master equation describing the non-unitary time-evolution of a density matrix representing the state of an open quantum system. This equation can be written as

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_{i=1}^{N^2-1} \gamma_i \left(A_i \rho A_i^\dagger - \frac{1}{2}\rho A_i^\dagger A_i - \frac{1}{2} A_i^\dagger A_i \rho \right), \tag{3.16}$$

where the first term represents the unitary part of the dynamics generated by the Hamiltonian and the operators A_i are usually referred to as Lindblad operators. A detailed proof that this equation defines the most general generator of a quantum dynamical semigroup for finite-dimensional systems has been given by Gorini, Kosakowski and Sudarshan [26], and independently by Lindblad [33].

This general master equation is mentioned here for completeness, but is not used in the model presented in this chapter. Instead, Section (3.2) presents a different approach by building up a chain of correlation functions for some dynamical map.

Let us briefly summarise the properties which this broad class of dynamical maps must satisfy:

- The map should be affine. This allows us to write a linear time evolution map
$$\Lambda(t) : \rho(0) \to \rho(t). \tag{3.17}$$
- The map should be positive, i.e., maps positive operators to positive operators.

- The map Λ should be trace-preserving. Equivalently, the dual map Λ^* in the Heisenberg picture should be unity-preserving.
- The map $\Lambda(t)$ should depend continuously on time, and it should be connected to the identity map such that $\Lambda(0) = \mathrm{id}$.
- It should be possible to extend the map to act on a larger space, composed of the original system plus an arbitrarily large ancillary space. That is, the map should be extendible to an affine transformation of some global state-space of the system and environment. This requirement is referred to as "complete positivity" of the map Λ, and is a very strong requirement.

This last requirement, complete positivity, is of particular importance. It is more than simply asking that the map is positive. Imagine a scenario where we have some system of interest embedded in some environment in such a way that they remain entirely disconnected from one another for all time. How does the time evolution of this reduced system then look? Since the system does not ever interact with the environment, it should make absolutely no difference whether this environment is taken into account or not. In other words, if we consider the action of the map Λ extended to some arbitrarily larger space, it should remain a positive map. More precisely, if we consider the map $\mathrm{id}_m \otimes \Lambda$ acting on a composite space consisting of the original system and some m-dimensional ancillary space, we should find that this extended map is positive no matter the dimension m of the ancillary space.

A commonly cited example of where things can go wrong is the transposition map, which is certainly a positive map since it leaves all eigenvalues invariant.

Consider the state of a pair of maximally entangled qubits, the Bell-state

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{3.18}$$

The density matrix for this two-qubit state is

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \tag{3.19}$$

or, writing it in a way which still illustrates the tensor structure,

$$\rho = \frac{1}{2}\begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix}. \tag{3.20}$$

To check whether it is a completely positive map, let us try and transpose only one of the two qubits. Such a map can be written as

$$(\mathrm{id}\otimes\mathrm{T})\rho = \frac{1}{2}\begin{pmatrix} \begin{pmatrix}1&0\\0&0\end{pmatrix}^{\mathrm{T}} & \begin{pmatrix}0&1\\0&0\end{pmatrix}^{\mathrm{T}} \\ \begin{pmatrix}0&0\\1&0\end{pmatrix}^{\mathrm{T}} & \begin{pmatrix}0&0\\0&1\end{pmatrix}^{\mathrm{T}} \end{pmatrix} \tag{3.21}$$

$$= \frac{1}{2}\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix}, \tag{3.22}$$

which clearly has a negative eigenvalue. The single-qubit transposition map already fails to remain positive when it is extended by the identity to act on an expanded space of two qubits.

A simple criterion for deciding whether or not a map is completely positive is related to the Choi-Jamiołkowski isomorphism. Choi's result states that for some given positive map $\Lambda : \mathbb{C}^{n\times n} \to \mathbb{C}^{m\times m}$, the following statements are equivalent:

- The map Λ is completely positive
- The matrix with operator entries

$$C_\Lambda = (\mathrm{id}_n \otimes \Lambda)\left(\sum_{i,j} E_{i,j}\otimes E_{i,j}\right) = \sum_{i,j} E_{i,j}\otimes\Lambda(E_{i,j}), \tag{3.23}$$

  henceforth referred to as the Choi encoding of a map, is positive.
- Λ is n-positive.

The Choi encoding provides a quick and convenient method for determining the conditions a map must satisfy in order to be completely positive. Later, it will also turn out to be a necessary ingredient in representing the actions of maps on states or operators.

3.1.3 Generalised pointer measurements

Before constructing the model in the next section, the final ingredient shall now be introduced. When a measurement is made, in the context of quantum systems,

it is traditionally a von Neumann measurement. This type of measurement, introduced in Chapter (1), is a direct measurement made on the state of the system in question. After such a measurement, the state of the measured system then collapses into the eigenspace associated with the measurement outcome.

In contrast to the von Neumann measurement scheme, one can also make a measurement using a so-called *unsharp observable* which has a discrete set of outcomes $\{\mu_i\}$. This observable corresponds to some apparatus, a measurement device, and this type of measurement is referred to as a generalised pointer measurement. The idea behind this kind of measurement is that if an observer wishes to make a measurement on the state of a quantum system, described by a Hilbert space $\mathcal{H}$, he/she should first introduce some measurement apparatus which then interacts with the system. It is through this interaction that the state of the apparatus and the state of the system become entangled in such a way that measuring the state of the apparatus results in an indirect measurement on the system itself. The pointer apparatus is itself a quantum system and is described by a Hilbert space $\mathcal{H}_A$ spanned by an orthonormal set of vectors $\{\phi_i\}$.

For the sake of this simplified argument, each vector ϕ_i corresponds to a particular outcome of the measurement,

$$\phi_i \Leftrightarrow \mu_i, \tag{3.24}$$

which in effect identifies a particular macrostate of the pointer apparatus with a corresponding basis vector in $\mathcal{H}_A$. Consequently, the apparatus must be macroscopic.

The initial composite state of the system and the apparatus is assumed to be a product (no entanglement exists),

$$\rho_C = \rho \otimes |\phi_0\rangle\langle\phi_0|, \tag{3.25}$$

where ρ_C is the density matrix describing the composite state, ρ is the density matrix describing the system to be measured and $|\phi_0\rangle$ is the ground-state, and initial state, of the apparatus. The initial state of the apparatus, $|\phi_0\rangle$, is the state to which it is reset before each measurement.

The interaction between the system and the apparatus is described by a unitary operator U acting on the composite space,

$$U = \sum_{j,k} u_{jk} \otimes |\phi_j\rangle\langle\phi_k|, \tag{3.26}$$

where $u_{jk} \in \mathcal{B}(\mathcal{H})$ and

$$\sum_k u_{ik} u_{jk}^\dagger = \delta_{ij} \mathbb{1}. \tag{3.27}$$

The final state of the composite system after interaction is then

$$\rho'_C = U\left(\rho \otimes |\phi_0\rangle\langle\phi_0|\right) U^\dagger \tag{3.28}$$

$$= \left(\sum_{j,k} u_{jk} \otimes |\phi_j\rangle\langle\phi_k|\right)\left(\rho \otimes |\phi_0\rangle\langle\phi_0|\right)\left(\sum_{l,m} u^\dagger_{lm} \otimes |\phi_m\rangle\langle\phi_l|\right) \tag{3.29}$$

$$= \sum_{j,k}\sum_{l,m} u_{jk}\,\rho\,u^\dagger_{lm} \otimes |\phi_j\rangle\langle\phi_k|\phi_0\rangle\langle\phi_0|\phi_m\rangle\langle\phi_l| \tag{3.30}$$

$$= \sum_{j,k}\langle\phi_k|\phi_0\rangle \sum_{l,m}\langle\phi_0|\phi_m\rangle\ u_{jk}\,\rho\,u^\dagger_{lm} \otimes |\phi_j\rangle\langle\phi_l| \tag{3.31}$$

$$= \sum_{j,l} u_{j0}\,\rho\,u^\dagger_{l0} \otimes |\phi_j\rangle\langle\phi_l| \tag{3.32}$$

Since we have assumed the apparatus is initially in the state $|\phi_0\rangle$, it suffices to label these terms with a single index and we can say $u_i = u_{i0}$ and

$$\rho'_C = \sum_{j,k} u_j\,\rho\,u^\dagger_k \otimes |\phi_j\rangle\langle\phi_k| \tag{3.33}$$

The state of the system being measured, found by taking the partial trace over the Hilbert space of the apparatus, can then be expressed as

$$\rho'_i = \frac{\Gamma_i(\rho)}{\operatorname{Tr}\Gamma_i(\rho)}, \tag{3.34}$$

where

$$\Gamma_i(\rho) := u_i \rho u_i^\dagger. \tag{3.35}$$

In the above expressions, ρ'_i is the state of the system after measurement outcome i, which occurs with probability $\operatorname{Tr}\Gamma_i(\rho)$.

This now defines a mapping $\Gamma := \sum_i \Gamma_i$ which takes an input state, the state of the system to be measured, and returns the final state of the system after measurement by the pointer apparatus but without selecting any outcome.

This pointer measurement, which defines what will be referred to as a model map Γ, combined with a completely positive dynamical map, Λ, forms the foundation for building a model of a quantum dynamical system in the following section.

3.2 Modelling dynamics using a half-chain

Spin chains are models which consist of a (possibly infinite) number of copies of a system, each connected with both the preceding and following site. Spin chains can be used to model ferromagnetism in statistical mechanics, where each site on the chain represents a site in a crystal lattice. Such models include the Lenz-Ising and Heisenberg models.

Another use for spin chains is to model dynamical systems, where each site on the chain represents the state of some system at some discrete time. An example of such a model is a discrete-time Markov chain. In this chapter, a discrete-time model of the dynamics of a spin system (a qubit being one example) is modelled using states on a half-chain.

Let us consider the scenario where we have some system, whose state living on the Hilbert space $\mathcal{H}_S$ is described by the density matrix ρ, coupled to an environment, on an ancillary space $\mathcal{H}_P$ with density matrix ω. The composite system at time $t = 0$ is prepared in the product state $\rho(0) \otimes \omega(0)$. The Hamiltonian governing the unitary evolution of this total system can be split into three terms,

$$H = H_S \otimes \mathrm{id}_P + \mathrm{id}_S \otimes H_P + \lambda V, \tag{3.36}$$

where the interaction term

$$V = \sum_\alpha V_\alpha^S \otimes V_\alpha^P. \tag{3.37}$$

We can then write the unitary time-evolution operator

$$U_t = \exp(-\mathrm{i}tH). \tag{3.38}$$

We can view this Hamiltonian dynamics on the level of the reduced system, the reduced dynamics, as a kind of black-box. This black-box dynamics of the reduced system, Λ_t, allows us to express two-time correlation functions as

$$\mathrm{Tr}\,(c\Lambda_t\rho) = \mathrm{Tr}\,(\Lambda_t^* c\rho) = \mathrm{Tr}\,[(c \otimes \mathbb{1}_P)U_t(\rho \otimes \omega)U_t^*] \tag{3.39}$$

for some arbitrary observable $c \in \mathcal{B}(\mathcal{H}_S)$, where Λ_t is as before, a linear completely-positive trace-preserving map in the Schrödinger picture and Λ_t^* is a linear completely-positive identity-preserving map in the Heisenberg picture:

$$\Lambda_t : \mathcal{H}_S \to \mathcal{H}_S,\ t \geq 0 \text{ and } \mathrm{Tr}\,(\Lambda_t\rho) = \mathrm{Tr}\,(\rho), \tag{3.40}$$

$$\Lambda_t^* : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S),\ t \geq 0 \text{ and } \Lambda_t^*\mathbb{1} = \mathbb{1}. \tag{3.41}$$

This has the consequence that any reduced evolution of the system is completely positive. The dynamics are such that it not only preserves positivity but also

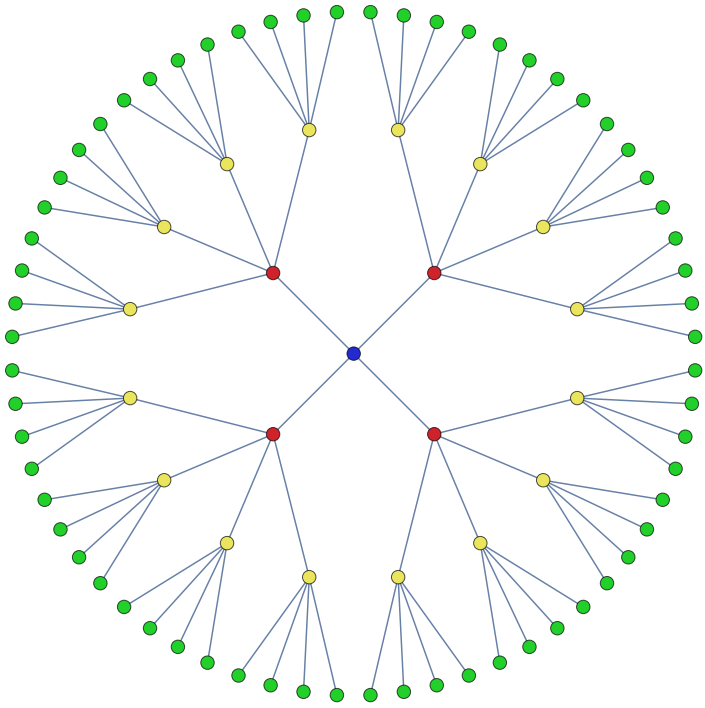

Figure 3.2: Half-chain model tree structure for a model with 4 partitions. The central blue circle represents the initial state, the reds the first site, the yellows the second site and the greens the third site.

positivity of any extended space, and as such the dynamics can be said to be completely positive.

Higher-order correlation functions are constructed in a rather particular fashion. The reason the ancillary space $\mathcal{H}_P$ has been introduced, is to use this as a pointer device for making pointer measurements as described in Section (3.1.3). Following the two-time correlation function given by

$$\text{Tr}\left[(a \otimes \mathbb{1}_P)U_t(\rho \otimes \omega)U_t^*(b \otimes \mathbb{1}_P)\right], \tag{3.42}$$

where we have factorised $c = ab$ for reasons which will become clear later on, the three-time correlation function can be written

$$\text{Tr}\left[(a_2 \otimes \mathbb{1}_P)U_{t_2-t_1}(a_1 \otimes \mathbb{1}_P)U_{t_1}(\rho \otimes \omega)U_{t_1}^*(b_1 \otimes \mathbb{1}_P)U_{t_2-t_1}^*(b_2 \otimes \mathbb{1}_P)\right], \tag{3.43}$$

and so on. What this is in effect doing, is letting the composite system evolve unitarily in discrete time steps between periodic pointer measurements through the interaction between the system and the ancillary space of the pointer measuring device. No measurement is made on the pointer system until after the final, n-th, timestep. The final pointer-measurement is made by the outermost trace operator, which returns a chosen multi-time correlation depending on the choice of observables $\{a_i, b_j | 1 \leq i, j \leq n\}$.

One may notice that the reduced dynamics are nothing more than a specific case of this particular hierarchy of multi-time correlation functions, in the above case by taking $a_2 = b_1 = b_2 = \mathbb{1}$.

Modeling a process in such a way allows for the straightforward computation of any/all multi-time correlation functions as a semi-infinite chain. We begin by specifying a state-space $\mathcal{S}(\mathcal{A})$, where $\mathcal{A}$ is a unital C^* algebra of observables and a completely positive affine map $\Lambda : \mathcal{S}(\mathcal{A}) \mapsto \mathcal{S}(\mathcal{A})$ which defines a unit-step in the dynamical system. The full dynamics is governed by the semigroup $\{\Lambda^n \mid n \in \mathbb{N}^0\}$ and properties such as its invariant state and the dynamical rate of convergence from some general state to the invariant state can be studied. Of specific interest is studying the dynamical entropy of such a model process. Dynamical entropy characterises the randomising properties of the dynamics.

3.2.1 Building the model

We wish to build a model for some dissipative dynamics on a finite system. For a d-dimensional quantum system, we have an algebra of observables $\mathcal{A}$, some completely-positive dynamical map Λ with Kraus decomposition

$$\Lambda(\rho) = \sum_{i=1}^{l} y_i \rho y_i^\dagger \tag{3.44}$$

and an associated reference-state σ which we will take to be the initial state of the system.

Here, the number of Kraus operators, l, can been chosen to be the square of the dimension of the density matrix ρ. Since ρ is a $d \times d$ matrix, any Kraus representation of a map from $\mathcal{M}_d$ to $\mathcal{M}_d$ with more than d^2 operators would be over-specified.

Given this dynamical system, the aim is to associate to it some measure of entropy. We do this by first modelling the dynamics in terms of a semi-infinite chain and then calculating the average entropy per site of the chain. To make the entropy measurement independent of the choice of model, the final step is to take the supremum of the average entropy over all possible choices of models.

To construct the model on the half-chain, the state-space of the system is partitioned using a set of k operators $\{x_i \in \mathcal{A} : i \in \mathbb{N}^0 \wedge i \leq k\}$ which are partitions of unity, analogous to the classical example,

$$\sum_{i=1}^{k} x_i^\dagger x_i = \mathbb{1}. \tag{3.45}$$

These partitions are nothing more than the Kraus operators corresponding to some model map Γ^*. The single-site density matrix of the chain generated by this model can be written as

$$\rho_1 = \sum_{i,j} \mathrm{Tr}\left[\sigma x_j^\dagger x_i\right] |i\rangle\langle j|. \tag{3.46}$$

The entries of the two-site density matrix can be written by letting the dynamics operate on the partition-observables,

$$[\rho_2]_{\substack{i_1,j_2\\ i_2,j_2}} = \mathrm{Tr}\left[\sigma x_{j_1}^\dagger \Lambda^*\left(x_{j_2}^\dagger x_{i_2}\right) x_{i_1}\right]. \tag{3.47}$$

The general form for the m-site density matrix is given by repeatedly applying the dynamical map to the partition-observables to generate a process in the form of a half-chain of length m,

$$[\rho_m]_{\substack{i_1,j_1\\ i_2,j_2\\ \vdots\\ i_{m-1},j_{m-1}\\ i_m,j_m}} = \mathrm{Tr}\left[\sigma x_{j_1}^\dagger \Lambda^*\left(x_{j_2}^\dagger \Lambda^*(\ldots \Lambda^*(x_{j_{m-1}}^\dagger \Lambda^*(x_{j_m}^\dagger x_{i_m}) x_{i_{m-1}}) \ldots) x_{i_2}\right) x_{i_1}\right]. \tag{3.48}$$

Since the dynamical map Λ^* is linear, it is easy to see that tracing over the last (mth) site exactly recovers the $(m-1)$-site density matrix. If we do this, by summing over all density matrices with elements defined as in Equation (3.48) where $i_n = j_n$ (since it is a sum over diagonal elements), we can see that the innermost terms reduce to the identity,

$$\sum_{i_m = j_m} \ldots \Lambda^*(x_{j_m}^\dagger x_{i_m}) \ldots \tag{3.49}$$

because of Equation (3.45) and the fact that Λ is an affine map. This immediately reduces to the expression for $\rho^{(m-1)}$.

Equation (3.48) now expresses a state on a half-chain $\rho_m \in \otimes^n \mathcal{M}_{d^2}$ which models the quantum dynamical system $(\mathcal{A}, \Lambda^*, \sigma)$ by means of a model-map Γ^* which serves to partition the state-space. This model-map is the pointer-measurement map defined in Section (3.1.3).

3.3 Entropy

When one speaks of quantum dynamical systems, a number of different scenarios come to mind. One such scenario, is a quantum system which is prepared at one location and transported to another where it will be measured. This is an example of how information might be encoded into a quantum state such that it may be transmitted to another party by physically sending the quantum state through some channel. A channel in this context is nothing more than a completely-positive trace-preserving map. The channel describes the evolution of the quantum state between the sender and receiver, or between preparation and measurement.

One extreme example is the identity channel, which perfectly transfers the prepared state unaltered to the receiver. In this case, there is no evolution whatsoever. A broader class of quantum channels can be described in terms of automorphic maps, where the evolution of the quantum state is unitary. In this case, the evolution is reversible and the entropy of the state does not change. Such channels are noiseless; no randomness is introduced into the system and knowing the input (prepared state), one can always perfectly predict the output. Broader still are the set of completely-positive trace-preserving maps. Such channels need not induce unitary dynamics and in general will cause an increase in entropy of the output state due to randomness introduced through interaction (entanglement) of the state with some noisy environment.

The model presented here corresponds to a noisy channel and the dynamics of the system is irreversible. Any input state will be randomised to a certain degree, and it is exactly this degree of randomisation which is of interest. In other words, it is interesting to characterise the rate of entropy production of quantum channels because this gives some measure of their randomising effects.

In order to characterise the entropy of the dynamical process, we will consider the second-order Rényi entropy. From Equation (2.2), the general form of the α-order Rényi entropy is given by

$$S_\rho(\alpha) = \frac{1}{1-\alpha} \log \operatorname{Tr} \rho^\alpha .$$

In calculating the Rényi entropy, we can use the replica-trick to express the trace of a power of a density matrix using Equation (2.4), which we rewrite here as

$$\operatorname{Tr} \rho^n = \operatorname{Tr} \left(\underbrace{\rho \otimes \rho \otimes \cdots \otimes \rho}_{n \text{ times}} \, T_n \right) , \tag{3.50}$$

where T_n is the cyclic shift operating on the n-fold tensor power of the original density matrix. Using this, we can express the nth-order Rényi entropy for the two-site half-chain as

$$S_{\rho_2}(n) = -\log \mathrm{Tr} \left(\left\{ \sum_{\substack{i_1,j_1 \\ i_2,j_2}}^{k} \left(|i_1\rangle\langle j_1| \otimes |i_2\rangle\langle j_2|\right) \mathrm{Tr} \left[\sigma x_{j_1}^\dagger \Lambda \left(x_{j_2}^\dagger x_{i_2} \right) x_{i_1} \right] \right\}^{\otimes n} T_n \right). \tag{3.51}$$

Higher order Rényi entropies are calculated in a similar fashion.

The construction of this half-chain model is such that the multi-time correlation functions are formed by a weaving of the initial state through the model and dynamical maps, Γ and Λ. Each weave through the maps generates a new site on the half-chain. In calculating the entropy generated, these two maps can be combined into a new map Δ, which combines this interleaving.

As a first step, consider this new map Δ in the case of the second-order Rényi entropy of a one-site chain. In this case, the entropy is

$$S_\rho(2) = -\log \mathrm{Tr} \left(\rho \otimes \rho T_2 \right), \tag{3.52}$$

where

$$\rho = \sum_{i,j} \mathrm{Tr}\, \sigma \Lambda(x_j^\dagger x_i) \otimes |i\rangle\langle j|. \tag{3.53}$$

This gives

$$S_\rho(2) = \sum_{k,l} \langle kl| \sum_{\substack{i_1,j_1 \\ i_2,j_2}} \left[\mathrm{Tr}\, \sigma \Lambda(x_{j_1}^\dagger x_{i_1}) \right] \left[\mathrm{Tr}\, \sigma \Lambda(x_{j_2}^\dagger x_{i_2}) \right] \otimes |i_1\rangle\langle j_1| \otimes |i_2\rangle\langle j_2| lk\rangle. \tag{3.54}$$

This simplifies to

$$S_\rho(2) = \sum_{k,l} \left[\mathrm{Tr}\, \sigma \Lambda(x_l^\dagger x_k) \right] \left[\mathrm{Tr}\, \sigma \Lambda(x_k^\dagger x_l) \right] \tag{3.55}$$

$$= \mathrm{Tr} \sum_{k,l} \left(\sigma \otimes \sigma\right) \left(\Lambda \otimes \Lambda\right) \left(x_l^\dagger \otimes x_k^\dagger \right) \left(x_k \otimes x_l \right) \tag{3.56}$$

$$= \mathrm{Tr} \sum_{k,l} \left(\sigma \otimes \sigma\right) \left(\Lambda \otimes \Lambda\right) \left(x_l^\dagger \otimes x_k^\dagger \right) T_2 \left(x_l \otimes x_k \right) T_2 \tag{3.57}$$

$$S_\rho(2) = \mathrm{Tr} \left(\sigma \otimes \sigma\right) \left(\Lambda \otimes \Lambda\right) \left\{ \left(\Gamma \otimes \Gamma\right) \left(T_2\right) T_2 \right\}. \tag{3.58}$$

In the same way, the third-order Rényi entropy for a one-site chain is

$$S_\rho(3) = \mathrm{Tr}\ (\sigma \otimes \sigma \otimes \sigma)\,(\Lambda \otimes \Lambda \otimes \Lambda)\,\{(\Gamma \otimes \Gamma \otimes \Gamma)\,(T_3)T_3\}\,. \tag{3.59}$$

Repeating these calculations for a two-site chain gives the entropies

$$S_\rho(2) = \mathrm{Tr}\ (\sigma \otimes \sigma)\,(\Lambda \otimes \Lambda)\,(\Gamma \otimes \Gamma)\,[(\Lambda \otimes \Lambda)\,\{(\Gamma \otimes \Gamma)\,(T_2)T_2\}\,T_2]\,T_2 \tag{3.60}$$

and

$$S_\rho(3) = \mathrm{Tr}\ \left(\sigma^{\otimes 3}\right)\left(\Lambda^{\otimes 3}\right)\left(\Gamma^{\otimes 3}\right)\left[\left(\Lambda^{\otimes 3}\right)\left\{\left(\Gamma^{\otimes 3}\right)(T_3)T_3\right\}T_3\right]T_3. \tag{3.61}$$

We can then explicitly define the action of this new map Δ for the nth-order Rényi entropy of a one-site chain as

$$\Delta_n(\cdot) = (\Lambda^{\otimes n})\left[(\Gamma^{\otimes n})(\cdot\ T_n)T_n\right]. \tag{3.62}$$

For a 2-site half-chain,

$$\Delta_n^2(\cdot) = \Delta_n\left\{(\Lambda^{\otimes n})\left[(\Gamma^{\otimes n})(\cdot\ T_n)T_n\right]\right\}, \tag{3.63}$$

and so on.

Consequently, the nth-order Rényi entropy for an m-site half-chain becomes

$$S_{\rho_m}(n) = -\log \mathrm{Tr}\,\Delta_n^m(T_n), \tag{3.64}$$

where ρ_m is the density matrix corresponding to an m-site chain, as given in Equation (3.48).

An important question to ask is whether the output entropy of such a map is bounded. That is, if we take the limit $m \to \infty$, does the average entropy of a site in the semi-infinite chain diverge?

Consider the identity-preserving completely positive map $\mathbb{G}$ on $\mathcal{A}$

$$\mathbb{G} : \mathcal{A} \to \mathcal{A} : z \mapsto \sum_{i=1}^{k} x_i^* z x_i\,. \tag{3.65}$$

Suppose that $\{y_\alpha\}$ is a size κ operational partition that generates the same $\mathbb{G}$:

$$\sum_{i=1}^{k} x_i^* z x_i = \sum_{\alpha=1}^{\kappa} y_\alpha^* z y_\alpha \quad \forall\ z \in \mathcal{A} \tag{3.66}$$

then there exists a unitary matrix u such that

$$y_\alpha = \sum_{i=1}^{k} u_{\alpha i}\, x_i \quad \forall\ \alpha\,. \tag{3.67}$$

We denote the density matrices of the model on a half-chain, with $\mathcal{M}_\kappa$ as the single-site algebra, defined by the partition $\{y_\alpha\}$ by τ. Then, the single-site, two-site, etc., density matrices are expressed as

$$\tau_1 = \sum_{\alpha,\beta=1}^{\kappa} \Big(\mathrm{Tr}_{\,\mathbb{C}^d} \sigma y_\beta^* y_\alpha\Big)\ |\alpha\rangle\langle\beta| \tag{3.68}$$

$$\tau_2 = \sum_{\alpha_1,\alpha_2,\beta_1,\beta_2=1}^{\kappa} \Big(\mathrm{Tr}_{\,\mathbb{C}^d} \sigma y_{\beta_1}^* \Lambda^*\big(y_{\beta_2}^* y_{\alpha_2}\big) y_{\alpha_1}\Big)\ |\alpha_1\rangle\langle\beta_1| \otimes |\alpha_2\rangle\langle\beta_2| \tag{3.69}$$

$$\vdots \tag{3.70}$$

Expressing the y_α as linear combination of the x_i one obtains

$$\tau_1 = \sum_{\alpha,\beta=1}^{\kappa} \sum_{i,j=1}^{k} \overline{u_{\beta j}} u_{\alpha i} \Big(\mathrm{Tr}_{\,\mathbb{C}^d} \sigma x_j^* x_i\Big)\ |\alpha\rangle\langle\beta| \tag{3.71}$$

$$= \sum_{i,j=1}^{k} \Big(\mathrm{Tr}_{\,\mathbb{C}^d} \sigma x_j^* x_i\Big) \Big(\sum_{\alpha=1}^{\kappa} u_{\alpha i}\,|\alpha\rangle\Big) \Big(\sum_{\beta=1}^{\kappa} \overline{u_{\beta j}}\,\langle\beta|\Big) \tag{3.72}$$

$$= u \Big(\sum_{i,j=1}^{k} \Big(\mathrm{Tr}_{\,\mathbb{C}^d} \sigma x_j^* x_i\Big)\ |i\rangle\langle j|\Big)\ u^\dagger \tag{3.73}$$

$$= u \rho_1 u^\dagger\,. \tag{3.74}$$

More generally:

$$\tau_m = \underbrace{u \otimes u \otimes \cdots \otimes u}_{m \text{ times}}\ \rho_m\ \underbrace{u^\dagger \otimes u^\dagger \otimes \cdots \otimes u^\dagger}_{m \text{ times}}\,. \tag{3.75}$$

Hence the entropies, Rényi or von Neumann, of ρ_m actually only depend on $\mathbb{G}$ and not on the chosen Kraus decomposition of $\mathbb{G}$. From now on we can therefore restrict ourselves to build models using operational partitions $\{x_i\}$ with at most d^2 elements as they will generate an arbitrary $\mathbb{G}$.

Next, we consider for any m an auxiliary system

$$\mathcal{M}_d \otimes \big(\mathcal{M}_k \otimes \mathcal{M}_\kappa\big)^{\otimes m} \tag{3.76}$$

with density matrix

$$\begin{aligned}\eta_m = \sum_{\substack{i_1,\dots,j_m=1\\ \alpha_1,\dots,\beta_m=1}}^{\kappa\ k} & x_{i_m} y_{\alpha_m} \cdots x_{i_1} y_{\alpha_1} \sigma y^*_{\beta_1} x^*_{j_1} \cdots y^*_{\beta_m} x^*_{j_1} \otimes \\ & |i_1\rangle\langle j_1| \otimes |\alpha_1\rangle\langle\beta_1| \otimes \cdots \otimes |i_m\rangle\langle j_m| \otimes |\alpha_m\rangle\langle\beta_m| \,.\end{aligned} \tag{3.77}$$

Because $\{x_i\}$ and $\{y_\alpha\}$ are partitions, the map

$$\begin{aligned} v_m : \mathbb{C}^d &\to \mathbb{C}^d \otimes \big(\mathbb{C}^k \otimes \mathbb{C}^\kappa\big)^{\otimes m} \\ &: \varphi \mapsto \sum_{\substack{i_1,\dots,i_m=1\\ \alpha_1,\dots,\alpha_m=1}}^{\kappa\ k} \big(x_{i_m} y_{\alpha_m} \cdots x_{i_1} y_{\alpha_1} \varphi\big) \otimes |i_1\rangle \otimes |\alpha_1\rangle \otimes \cdots \otimes |i_m\rangle \otimes |\alpha_m\rangle \end{aligned} \tag{3.78}$$

satisfies

$$\big(v_m\big)^\dagger v_m = \mathrm{id}_d \,. \tag{3.79}$$

Therefore η_m and σ have, up to multiples of 0, the same eigenvalues.

We can now use the triangle inequality for the von Neumann entropy to estimate the entropy of the model density matrix ρ_m. We observe that ρ_m is the reduction of η_m to the subsystem $\big(\mathbb{C}^k\big)^{\otimes m}$. Using the bipartite decomposition

$$\mathbb{C}^d \otimes \big(\mathbb{C}^k \otimes \mathbb{C}^\kappa\big)^{\otimes m} = \Big(\mathbb{C}^d \otimes \big(\mathbb{C}^\kappa\big)^{\otimes m}\Big) \otimes \big(\mathbb{C}^k\big)^{\otimes m} \tag{3.80}$$

and the bound $S \leq \log D$ for a density matrix of dimension D this leads to

$$S\big(\rho_m\big) \leq S\big(\eta_m\big) + \log d + m \log \kappa = 2 \log d + m \log \kappa \,. \tag{3.81}$$

Therefore the average von Neumann entropy of our model $\big\{\rho_m\big\}$ is bounded above by $\log \kappa$. In particular, a finite dimensional reversible dynamical system always has zero average entropy. It is only because a dynamical map is dissipative, $\kappa > 1$, that we can possibly obtain a non-zero average entropy. In the following chapter we will illustrate this possibility for a particular class of dissipative qubit maps. Clearly, the monotonicity of the Rényi entropies in their order implies that also all averages Rényi entropies of order greater than 1 are bounded by $\log \kappa$.

Although the upper bound on the average entropy does not depend on the choice of model, the average entropy itself certainly does. In order to remove this dependence of the average entropy on the chosen model, we take the supremum over all models,

$$s(\rho) = \sup_{\Gamma} \lim_{m\to\infty} \frac{1}{m} S(\rho_m). \tag{3.82}$$

Looking back to equation (3.64), now having assurance that the average entropy will not diverge as the chain grows, we can ask more questions about the average entropy in the half-chain model. The average entropy, calculated in the limit $m \to \infty$, is certainly governed by the largest eigenvalue of the map Δ.

A natural question one may ask is "What is the maximum entropy rate for such a model?" Stated differently, "How can the partitioning in Equation (3.45) best be chosen such that they result in the maximum average entropy?"

It is evident from Equation (3.64) that in order to maximise the entropy, the largest eigenvalue of Δ should be minimised with respect to the choice of partitions. In general, this is a difficult problem since the dimensions of Δ grows exponentially with the order n and the map is not Hermitian.

Additionally, the density matrix for the half-chain also grows in dimension exponentially in m, although it does have a very sparse fractal-like structure when we restrict ourselves to Davies-type maps [16], as we shall see in the example to follow. We will attempt to investigate this question in the following chapter with the help of a specific example, the dynamics of a qubit system.

3.4 Conclusion

The question of how general open quantum systems evolve in time is both very interesting and at the same time very difficult to answer. It is interesting because at the microscopic scale, systems behave according to the laws of quantum mechanics and a deeper understanding of these systems allows us to develop new techniques for manipulating and predicting the behaviour of the world at the atomic scale.

Although a general description of open quantum dynamics remains elusive, restricting the problem to smaller simpler models through strong assumptions or approximations can yield useful and sometimes surprising results. Readers looking for a comprehensive treatment of dynamics in quantum systems may refer to [1, 13]

The goal of this chapter was to develop a scheme which can be used to model the dynamical entropy for reduced systems undergoing dissipative dynamics. This scheme modelled the reduced dynamics by building up a semi-infinite half-chain of multi-time correlation functions where each site on the chain is labelled by discrete time slices. Using this model, one can calculate firm bounds on the entropy production rate of the underlying process. Later, a general expression was derived for the Rényi entropy production rate of any order.

The scheme presented here does not make any additional assumptions on the dynamics beyond what was discussed in Section (3.1.2), namely, the dynamical map is completely positive, trace preserving and can be written in Lindblad form. For practical purposes, it will be neccessary to make some other strong assumptions in the example to follow.

Since the average entropy is governed by the largest eigenvalue of the matrix representing the site-generating map Δ, it is in general not possible to explicitly compute since the dimensions of such symbolic matrices are very large. In the following chapter, a low-dimension example is explored where the dynamical map is of a special type which does not mix the diagonal and off-diagonal elements of density matrices. This will allow us to generate explicit results to illustrate this modelling technique.

Chapter 4

Modelling qubit dynamics

In the previous chapter, a theoretical description of a semi-infinite spin chain model of a quantum dynamical system was presented. It remained quite general, only requiring an autonomous system evolving under Hamiltonian dynamics which is periodically probed using generalised pointer measurements to build up multi-time correlation functions.

However, as the dimensions of the system grow the characterisation of the model system's entropy rate rapidly becomes a very difficult problem because the average entropy is determined by the dominant eigenvalue of the map Δ in Equation (3.64). If we limit ourselves to modelling the dynamics of a system of low dimension and carefully choose the right kind of dynamical map Λ, the problem should remain reasonably manageable.

In this chapter, a specific example is investigated - a qubit system evolving under a very specific class of dynamical map, the Davies maps. The difficulties mentioned in the closing of the previous chapter of tackling high-dimensional systems is avoided here by studying the simplest possible system, one with just two-levels. This allows explicit and exact calculations to be performed, which would otherwise rapidly become intractable with growing dimensions. This qubit example, despite being a very simple system, is a clear example of a non-Markovian quantum process which reduces to a Markovian process in the classical limit.

4.1 A note on representations

Before introducing the qubit model it is necessary to first become familiar with a convenient way to write down the actions of maps on operators and find a good representation of these various objects in terms of matrices.

A matrix X with elements X_{ij}, where $\{i, j \in \mathbb{N} | 1 < i, j \wedge i \leq N \wedge j \leq M\}$ can be reshaped by reordering the elements into a vector $\vec{x}_k$ of dimension $N \times M$ such that $\vec{x}_k = X_{ij}$, where $k = (i-1)\,N + j$. This reshapes a rectangular matrix into a column vector where the elements are lexicographically (row-by-row) ordered. This reshaping is the usual way of defining a (usually square) dynamical map acting on some operator in terms of a multiplication of a matrix with a vector.

Suppose we have some two-dimensional operator

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \tag{4.1}$$

upon which acts some map Φ. Reshaping the elements of A into the vector $\vec{a}$, we can write $\Phi(A)$ as the product

$$\begin{pmatrix} \Phi_{11} & \Phi_{12} & \Phi_{13} & \Phi_{14} \\ \Phi_{21} & \Phi_{22} & \Phi_{23} & \Phi_{24} \\ \Phi_{31} & \Phi_{32} & \Phi_{33} & \Phi_{34} \\ \Phi_{41} & \Phi_{42} & \Phi_{43} & \Phi_{44} \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{pmatrix}, \tag{4.2}$$

where the elements Φ_{ij} are determined by their actions on the unit vectors $\vec{e}_i$. Reshaping this product back into its original form yields

$$\begin{aligned} [\Phi(A)]_{11} &= \Phi_{11}a_{11} + \Phi_{12}a_{12} + \Phi_{13}a_{21} + \Phi_{14}a_{22} \\ [\Phi(A)]_{12} &= \Phi_{21}a_{11} + \Phi_{22}a_{12} + \Phi_{23}a_{21} + \Phi_{24}a_{22} \\ [\Phi(A)]_{21} &= \Phi_{31}a_{11} + \Phi_{32}a_{12} + \Phi_{33}a_{21} + \Phi_{34}a_{22} \\ [\Phi(A)]_{22} &= \Phi_{41}a_{11} + \Phi_{42}a_{12} + \Phi_{43}a_{21} + \Phi_{44}a_{22}. \end{aligned} \tag{4.3}$$

If one tries to use this reshaping to write down the action of maps acting on composite spaces, things quickly go wrong as can immediately be seen in the comparison

$$\overrightarrow{x \otimes y} \neq \vec{x} \otimes \vec{y} \tag{4.4}$$

because the tensor product disturbs the lexicographical ordering of the elements. The elements in this tensor product will need to be reordered in order to preserve this lexicographical ordering.

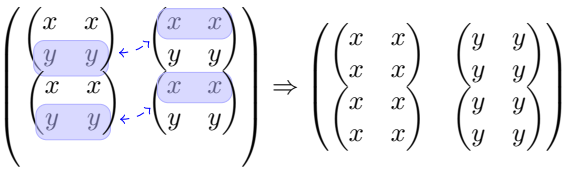

Figure 4.1: Illustration of a reshuffling of a two-fold tensor product of qubit operators

Consider the matrix $C = A \otimes B$ representing some operator acting in a composite space. We can express the elements of C as

$$C_{\substack{n\nu \\ m\mu}} = A_{mn} B_{\mu\nu}. \tag{4.5}$$

Alternatively, for an $m \times n$ matrix A and an $s \times t$ matrix B one can write the $ms \times nt$ matrix $C = A \otimes B$ as

$$C_{\alpha\beta} = A_{ij} B_{kl}, \tag{4.6}$$

where $\alpha = u(i-1) + k$ and $\beta = t(j-1) + l$.

In order to preserve the lexicographical ordering of elements, we first perform the reshuffling

$$C^R_{\substack{n\nu \\ m\mu}} = C_{\substack{nm \\ \nu\mu}} \tag{4.7}$$

before reshaping. To perform the reverse operation, we simply reshuffle again after reshaping back into a matrix, since $\left(C^R\right)^R = C$.

We now have a way to lexicographically reorder and reshape such that

$$\Gamma(\rho) \otimes \Gamma(\rho) = (\Gamma \otimes \Gamma)(\rho \otimes \rho).$$

A keen-eyed reader may notice at this point that the reshuffling described in Equation (4.7) is an instance of the Choi-encoding from Equation (3.23).

This reshuffling works for 2-fold composite spaces, but what if we take an n-fold tensor product of maps operating on some n-composite space?

The correct way to represent such an action whilst preserving the proper ordering of elements is to perform a series of reshufflings nested through the various levels of the tensor structure. For an n-fold tensor-product structure on the level of the map, one requires $n-1$ reshufflings, one between each of the adjacent tensor structure pairs. For a qubit map, the 2-fold tensor product of operators have the structure of a 2×2 matrix with each element itself also a 2×2 matrix. An

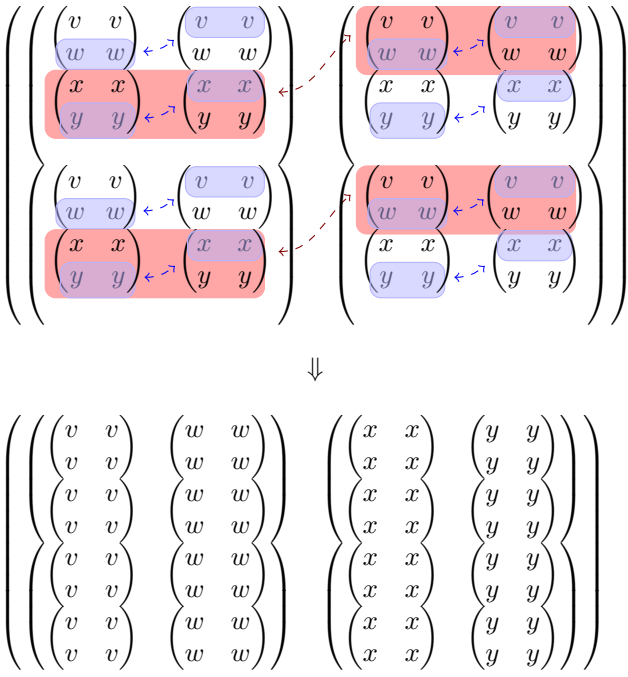

Figure 4.2: Illustration of a reshuffling of a three-fold tensor product of qubit operators

example of such a reshuffling is illustrated in Figure (4.1), where the marked entries are exchanged. The entries "x" and "y" are meaningless and intended solely to aid in visualising the structure.

The 3-fold tensor product of qubit operators is a lot more interesting. Here, there are two sets of reshufflings required. These reshufflings are illustrated in Figure (4.2), where the indicated elements are exchanged by the Choi-encoding and the entries "v", "w", "x" and "y" are intended purely to illustrate the structure. It should be noted that the order in which one performs the various exchanges of elements in the reshuffling does not affect the result, reshuffling between any particular tensor-product pair commutes with any reshuffling between any other chosen pair. This is a direct consequence of the associativity of tensor products. Figure (4.2) illustrates an example of a 3-fold tensor structure reshuffling, resulting in a matrix representation consistent with the scheme outlined in Equation (4.2).

Higher-order (n-fold) tensor-product structures are reshuffled by exchanging the relevant entries in each of the $n-1$ adjacent copies in exactly the same way.

4.2 A model for a two-level quantum system: The qubit

In this example, we consider a qubit with an associated dynamical map Λ^* which is a Davies-type map. In general, a Davies map satisfies the following properties:

- The map is completely positive, ensured by the positivity of the Choi-encoding.
- The map does not mix diagonal components of the density matrix with off-diagonals. The map therefore has a block-structure, where the diagonal mixing is stochastic and the off-diagonal evolution is dissipative.
- The map satisfies the detailed balance condition, which restricts the stochastic block to elements which satisfy $T_{i,j}\mu_i = T_{j,i}\mu_j$, where $T_{i,j}$ are elements of the stochastic block and μ_i is an element of the invariant measure. This is automatically satisfied in the qubit example presented here.
- The map is a one-parameter semigroup generated by $\exp(\mathcal{G}t)$, where $\mathcal{G}$ is of Lindblad-type. This is equivalent to requiring that the Choi encoding of the map is positive in the subspace orthonormal to the maximally-entangled state [45].

The reason Davies maps are chosen for the dynamics is because although they are quantum maps, they do feature some properties similar to classical systems. Diagonal elements of density matrices are mixed stochastically and the off-diagonal elements decay, there is never a mix between the diagonal and off-diagonal elements. This very special structure of this class of maps introduces some additional symmetries into the model, allowing us to avoid some complications in the explicit calculations.

Since this type of map leaves the identity operator invariant, it will, on average, increases a state's entropy monotonically [43]. This means that the entropy production of a Davies map is maximised when the off-diagonal block of the map is zero - i.e., it decays the off-diagonals of the density matrix immediately. Conversely, if the off-diagonals are as large as possible, within the bounds we will discover shortly, the entropy will increase very slowly.

Consider the qubit system whose dynamics are governed by the completely positive dynamical map

$$\Lambda = \begin{pmatrix} 1-\alpha & 0 & 0 & \alpha \\ 0 & \gamma & 0 & 0 \\ 0 & 0 & \gamma^* & 0 \\ \beta & 0 & 0 & 1-\beta \end{pmatrix}. \tag{4.8}$$

Here, we have used the usual representation outlined earlier in Section (4.1).

We restrict the class of dynamical maps to Davies maps. Complete positivity requires that

$$1 > \alpha > 0, \quad 1 > \beta > 0 \quad \text{and} \quad |\gamma|^2 < 1 - \alpha - \beta + \alpha\beta. \tag{4.9}$$

The additional constraint

$$1 - \alpha - \beta > 0 \tag{4.10}$$

is needed in order to ensure that this map comes from a one-parameter semigroup connected to the identity.

What this means, is that the dynamical map can be expressed as

$$\Lambda = \exp L, \tag{4.11}$$

where L is called the *generator* of the dynamics (see [2] for more on this topic) such that

$$\frac{d}{dt}\rho_t = L\rho_t. \tag{4.12}$$

For our chosen dynamical map, this means that one of the eigenvalues of the generator L is $\log(1-\alpha-\beta)$ and leads to the condition in Equation (4.10).

The state-space of this qubit system, the C^* algebra of observables $\mathcal{S}(\mathcal{A})$, can be divided by taking k operational partitions of identity in $\mathcal{A}$:

$$\mathbf{X} = \{x_1, x_2, \ldots, x_k\} \text{ where } x_i \in \mathcal{A} \text{ and } \sum_{i=1}^{k} x_i^* x_i = \mathbb{1}. \tag{4.13}$$

This partitioning is used as a kind of weak measurement to probe the system, and defines what we call the model map Γ, where

$$\Gamma(\cdot) = \sum_{i=1}^{k} x_i^* \cdot x_i. \tag{4.14}$$

In this example, a partition is chosen in such a way that the resulting model map does not mix diagonal elements with off-diagonal elements. Instead, it

decays the off-diagonal terms and mixes diagonal elements stochastically. It then takes the form

$$\Gamma = \begin{pmatrix} 1-a & 0 & 0 & a \\ 0 & c & 0 & 0 \\ 0 & 0 & c^* & 0 \\ b & 0 & 0 & 1-b \end{pmatrix}. \tag{4.15}$$

Complete positivity of Γ requires that

$$1 > a > 0, \quad 1 > b > 0 \quad \text{and} \quad |c|^2 < 1 - a - b + ab. \tag{4.16}$$

An additional restriction analogous to Equation (4.10) for the map Λ is not present here since the model map is not a dynamical map.

A set of Kraus operators corresponding to the map Γ can be found by taking each of the four eigenvectors of the Choi encoding of Γ, rescaling them by the square-root of the corresponding eigenvalue and reshaping them into square matrices. Completing this procedure, we find that the four Kraus operators are

$$x_1 = \begin{pmatrix} 0 & \sqrt{a} \\ 0 & 0 \end{pmatrix} \qquad x_2 = \sqrt{r_+} \begin{pmatrix} \begin{pmatrix} \dfrac{b-a+q}{2c^*} \end{pmatrix} & 0 \\ 0 & 1 \end{pmatrix}$$

$$x_3 = \begin{pmatrix} 0 & 0 \\ \sqrt{b} & 0 \end{pmatrix} \qquad x_4 = \sqrt{r_-} \begin{pmatrix} \begin{pmatrix} \dfrac{b-a-q}{2c^*} \end{pmatrix} & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.17}$$

where

$$q = \sqrt{(a-b)^2 + 4|c|^2}$$

and

$$r_\pm = 1 - \frac{1}{2}(a + b \pm q).$$

With the dynamical and model maps defined in Equations (4.8) and (4.15) respectively, using the procedure outlined earlier it is a simple matter to calculate the matrix elements for the map Δ_n. The problem of choosing the partitions which maximise the entropy production now reduces to minimising the largest eigenvalue of Δ with respect to the free parameters in Γ; i.e., minimising over a, b and c. Given the high dimensions, 4^n for the nth-order Rényi entropy, it helps to look at each of the independent blocks separately.

Armed with a way to represent these multi-dimensional objects, it is now possible to explicitly calculate each element of a matrix representation of the relevant

map Δ which describes the action of weaving the cyclic-shift operator T_n through m instances of the dynamical map Λ and the model map Γ. With this, we can explicitly express the nth-order Rényi entropy of an m-site half-chain using Equation (3.64):

$$S_{\rho_m}(n) = -\log \operatorname{Tr} \Delta_n^m(T_n).$$

The fact that we are able to find a matrix which encodes all the information about the entropy production of our model process is critical, as this reduces the problem of finding the maximum entropy produced by the process to finding and minimising the largest eigenvalue of said matrix. For constructing a model of a k-level system (where the system is described by a $k \times k$ density matrix), Δ_n is a square, usually non-Hermitian $k^{2n} \times k^{2n}$ matrix. Since this matrix grows in dimension exponentially with order n, we will limit ourselves to orders 2 and 3, although the procedure remains completely general for all higher orders.

Even for the simplest example of the second-order Rényi entropy in the case of a qubit model, the matrix Δ_2 is 16×16 and is not Hermitian. Nonetheless, it fortunately has a lot of structure due to the restrictions on the original model and dynamical maps. Something that may be immediately evident is that Δ_m has a block structure. That is, it can be decomposed into a number of independent blocks such that it factorises into a set of commuting sub-maps each acting on a different subspace. This greatly simplifies the search for the largest eigenvalue.

One of these blocks, or factors, is particularly interesting. The block with largest dimension acts on the space of cyclic permutations, introduced earlier in Equation (3.50). This block also turns out to be the only non-zero block in the Markovian limit, when the off-diagonal decay-rates of the model and dynamical maps become infinite.

4.3 Second-order Rényi entropy density

Consider first the second-order Rényi entropy for the qubit model. Using the usual representation, we can calculate each element of the matrix representation of the map Δ_2, pictured in Figure (4.3). After a careful inspection, one immediately notices that Δ_2 is composed of a single 6×6 block, two 4×4 blocks, and two 1×1 blocks. After exchanging the rows and columns we can rewrite this matrix in a block-diagonal form, shown in Figure (4.4), which makes this block structure much more evident.

The 1×1 blocks are trivially minimised by setting $c = \gamma = 0$. The 4×4 blocks are equivalent up to a unitary transformation (one which cyclically permutes

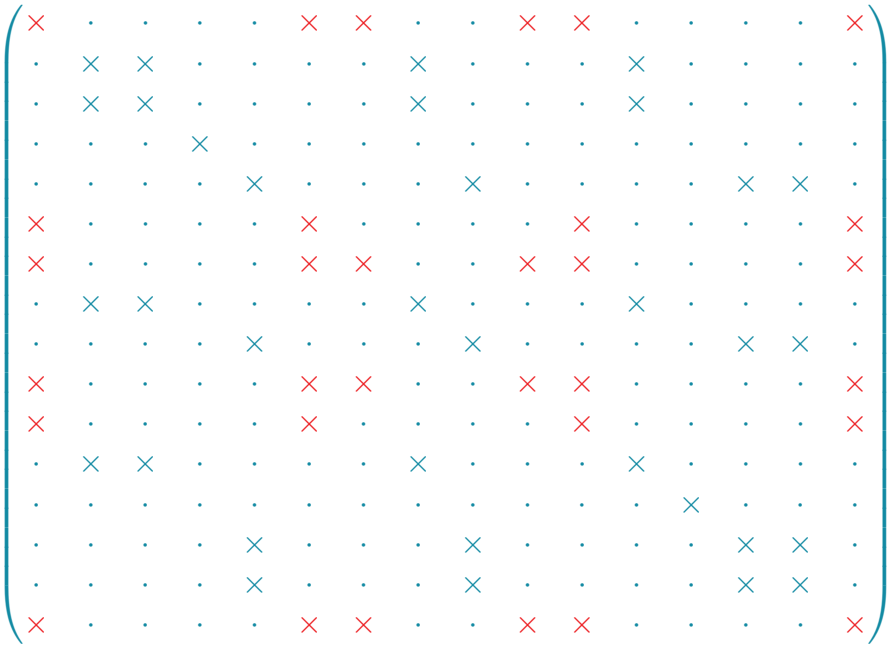

Figure 4.3: Matrix representation of Δ_2, where dots represent a zero element and a $\times$ represents a non-zero element. Elements coloured in red belong to the 6-by-6 block which acts on the T_2 subspace.

the rows and columns by one place each), and the eigenvalues can be computed explicitly.

The 6×6 block is the most interesting. Since this is the block which acts on the T_n operator from equation (3.64), it is the only block of Δ which is relevant. Its eigenvalues cannot be computed explicitly but because of the conditions imposed on Γ and Λ, every element of this block is non-negative. These six eigenvalues are depicted numerically in the three figures which follow, Figures (4.5-4.7). The largest eigenvalue can be found using the following formula from Perron-Frobenius theory:

Formula 1 (Collatz-Wielandt)**.** The Perron root of $A_{n\times n} > 0$ is found by

$$r = \max_{x \in \mathcal{N}} f(x),$$

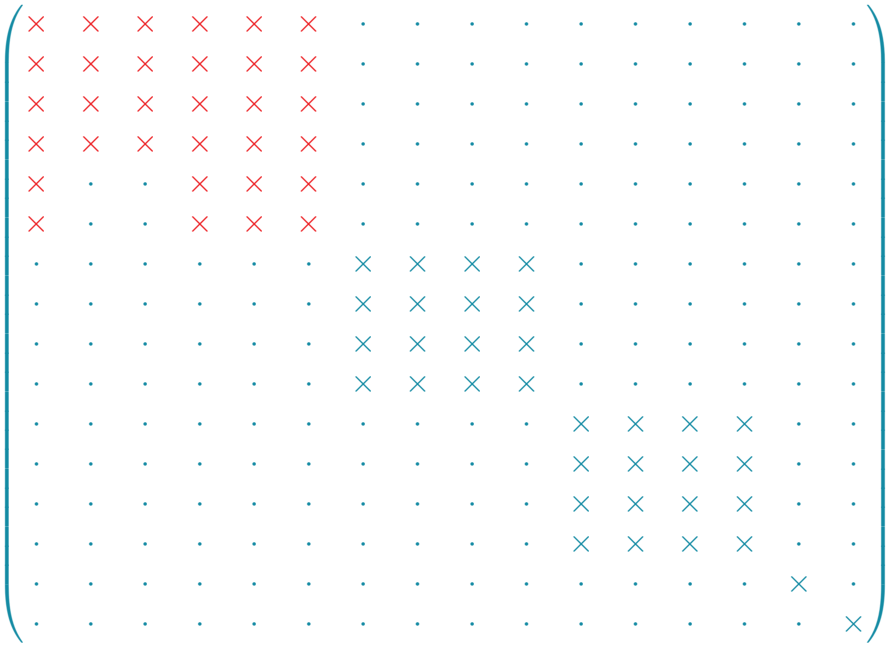

Figure 4.4: Matrix representation of Δ_2 with rows and columns reshuffled to make the block structure evident. Dots represent a zero element and a $\times$ represents a non-zero element. Elements coloured in red belong to the 6-by-6 block which acts on the T_2 subspace.

where

$$f(x) = \min_{\substack{1\leq i\leq n \\ x_i\neq 0}} \frac{[Ax]_i}{x_i} \text{ and } \mathcal{N} = \{x | x \geq 0 \text{ and } x \neq 0\}.$$

Performing this optimisation subject to the conditions (4.9), (4.10) and (4.16) gives the result that the largest eigenvalue is minimised when $c = 0$. A numerical plot around $c = 0$ for some randomly chosen parameters is shown in Figure (4.5). If the model map was under the same restrictions as the dynamical map, namely demanding that it is a one-parameter semigroup connected to the identity, the same argument as in Section (4.2) would apply and hence entropy would be maximised for $c = 0$.

After determining the optimal value for c, the remaining parameters should

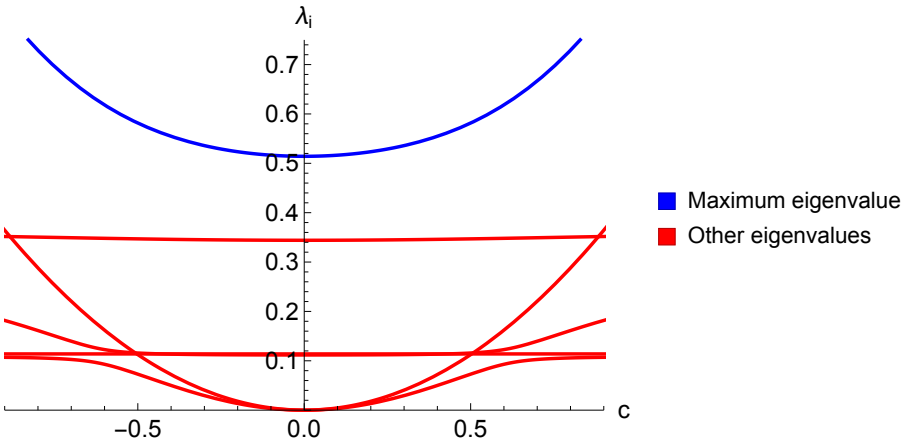

Figure 4.5: The six eigenvalues λ_i corresponding to the 6×6 block of the map Δ as a function of c with fixed parameters $a = 0.40$, $b = 0.15$, $\alpha = 0.356$, $\beta = 0.194$ and $\gamma = -0.375$.

also be optimised in a similar way, although it is not possible to express this optimal choice algebraically in closed form. A numerical plot is shown in Figure (4.6) depicting, for a particular choice of dynamical parameters, a maximum in entropy at a point near the boundary where $a = b$.

Another question which naturally arises is the behaviour of the entropy around $\gamma = 0$. One would expect that the entropy is maximised in the Markovian limit and should decrease as γ moves away from zero. This can indeed be seen in Figure (4.7), a numerical plot about $\gamma = 0$, which shows a monotonic decrease in entropy as $|\gamma|$ increases from zero for a set of randomly chosen parameters.

Setting $\gamma = 0$ means that the off-diagonal elements of the density matrix are killed off immediately. The only remaining dynamics is that of stochastic mixing of the diagonal elements which reminds us of the classical scenario. In fact, setting $c = 0$ in the model map Γ and $\gamma = 0$ in the dynamical map Λ results in every element outside the 6×6 block of the Δ map being zero. This is the Markovian limit and the resulting density matrix for the chain of arbitrary length m, ρ_m, is diagonal with full rank and maximises the entropy as expected.

When γ is as large in magnitude as possible, saturating the bound given in Equations (4.9), we expect a lower entropy as shown in Figure (4.7). This is reasonable because a larger gamma leads to a slower rate of decay of the off-diagonal terms in the density matrix. The only possible map corresponding

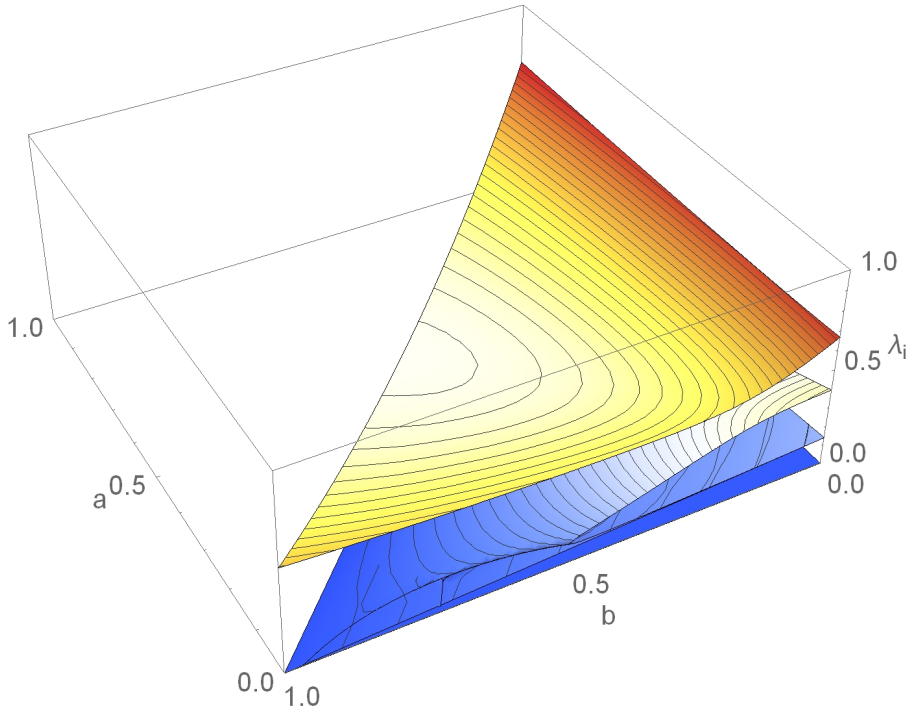

Figure 4.6: A contour plot of the six eigenvalues λ_i corresponding to the 6×6 block of the map Δ as a function of a and b with fixed parameters $c = 0$, $\alpha = 0.356$, $\beta = 0.194$ and $\gamma = -0.375$.

to non-decaying off-diagonals is when $\gamma = 1$ and $\alpha = \beta = 0$, the identity map.

4.4 Higher-order numerical example

With the aid of a numerical example, let us examine both the second and third-order entropy densities for qubits. We begin by explicitly defining a dynamical map, making sure that it indeed satisfies the constraints given in Equations (4.9-4.10).

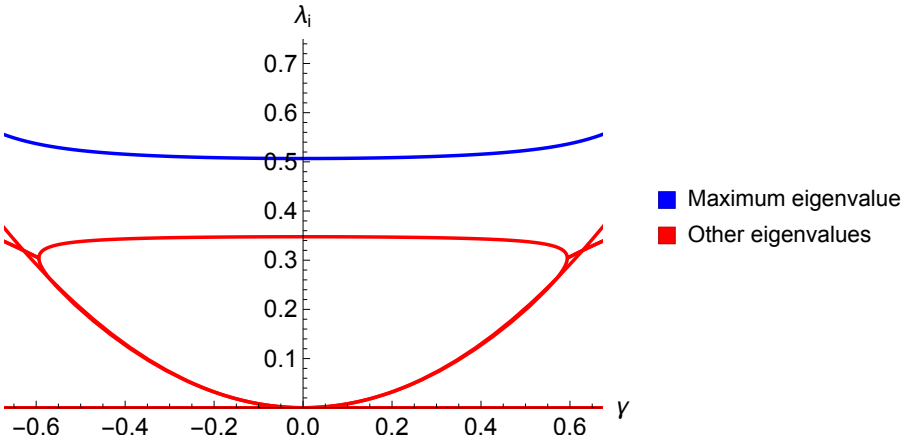

Figure 4.7: The six eigenvalues λ_i corresponding to the 6×6 block of the map Δ as a function of γ with fixed parameters $a = 0.40$, $b = 0.15$, $\alpha = 0.356$, $\beta = 0.194$ and $c = 0$, for all allowed values of γ within the bound given in Equation (4.9).

Picking values at random, we define our dynamical map as

$$\Lambda = \begin{pmatrix} 0.725 & 0 & 0 & 0.275 \\ 0 & 0.125 & 0 & 0 \\ 0 & 0 & 0.125 & 0 \\ 0.175 & 0 & 0 & 0.825 \end{pmatrix} \tag{4.18}$$

and the model map, which should later be optimised with respect to the dynamical map, is of the form given in Equation (4.15):

$$\Gamma = \begin{pmatrix} 1-a & 0 & 0 & a \\ 0 & c & 0 & 0 \\ 0 & 0 & c^* & 0 \\ b & 0 & 0 & 1-b \end{pmatrix}. \tag{4.19}$$

The dynamical map is defined by setting $\alpha = 0.275$, $\beta = 0.175$ and $\gamma = 0.125$ in Equation (4.8). Following the method detailed in Section (4.3), we easily confirm that $c = 0$ optimises the model map.

Maximising the second-order average Rényi entropy over the two remaining parameters a and b, we find that the optimal model map is defined by $a = 0.457$, $b = 0.543$ and $c = 0$.

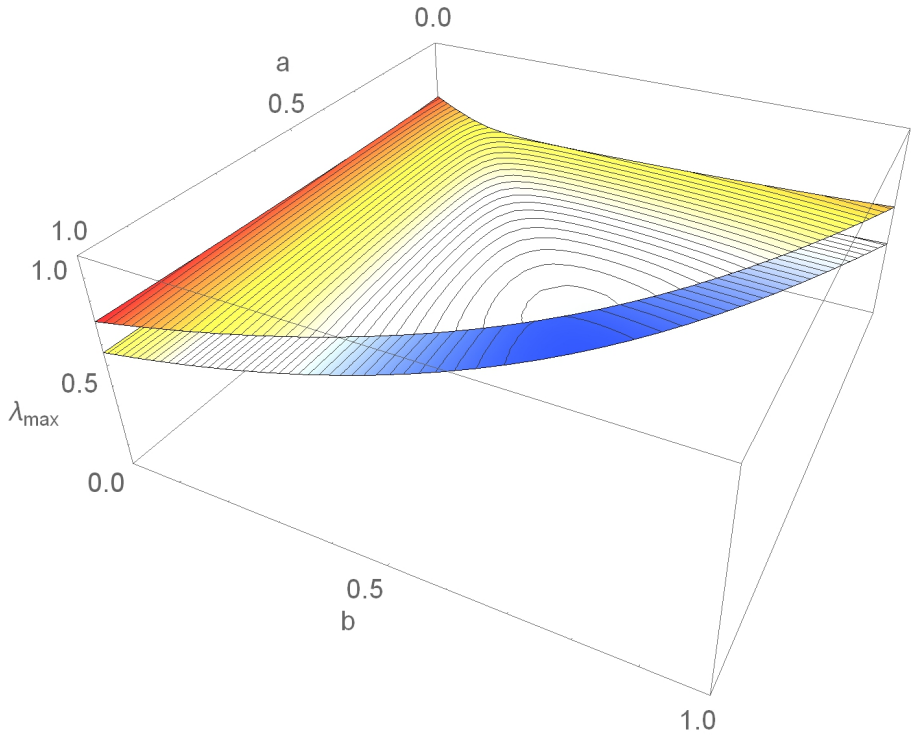

Figure 4.8: A contour plot of the largest eigenvalues of the maps Δ_2 (the upper layer, yellow-red) and Δ_3 (the lower layer, blue-yellow) as a function of a and b with fixed parameters $c = 0$, $\alpha = 0.275$, $\beta = 0.175$ and $\gamma = 0.125$.

We can repeat this for the third-order average Rényi entropy by using the map Δ_3 instead of Δ_2. In this case, we again conclude that the model map is optimised by choosing $a = 0.457$, $b = 0.543$ and $c = 0$. This is to be expected since the optimal choice of model map depends exclusively on the dynamics and not on the choice of Rényi entropy order.

Figure (4.8) depicts a surface plot of the largest eigenvalues of the maps Δ_2 and Δ_3, associated with the second and third-order average Rényi entropies respectively. In this figure, one can see that the two surfaces are non-intersecting, a consequence of the monotonicity of the Rényi entropy in order, and that the points corresponding to the minimum of each surface are at the same (a, b).

If one is explicitly given a dynamical map for an n-level system, it is a simple task to numerically optimise the corresponding model map. Using this model

map, calculating any integer-order average Rényi entropy is relatively simple.

4.5 Conclusion

The goal of this chapter was to apply the abstract model developed previously, in Chapter 3, to the simplest non-reversible dynamical system, a qubit undergoing dissipative dynamics with quantum detailed balance.

The example presented in this chapter is that of a two-level system with dynamics induced by a Davies map. These maps are dissipative but still useful in that it is still possible to make many explicit calculations, avoiding often intractable complications inherent to more general dynamics. Davies-type dynamics has the added property of being somewhat more classical in nature, and in certain limits can recover a classical behaviour.

In exploring the example presented here, some expected results were obtained. Namely, that the classical limit of destroying the off-diagonal terms in the relevant density matrices results in a maximum average entropy and that the Markovian limit of the model process similarly maximises the average entropy.

Whilst the model itself is in general not restricted to any particular choice of dynamics or any specific type of model map, the choices made in this chapter are primarily for ease of calculation only. Additionally, although the entropy usually studied is the von Neumann entropy, this chapter explores the average Rényi entropy and this again is for ease of calulations. One might then use a similar approximation scheme to Chapter 2 in order to recover the average von Neumann entropy.

Chapter 5

Concluding remarks

The goal of this thesis has been to investigate correlations and their dynamics in the context of quantum systems. A central idea throughout this work has been investigating the entropy of quantum systems. This is important for many applications, including characterising the information-carrying capacity of quantum channels and measuring the degree of entanglement of pure states.

In Chapter 2, the focus was on exploring the connection between the von Neumann entropy and integer-order Rényi entropies of quantum systems. An approximation scheme was developed for expressing the von Neumann entropy in terms of an arbitrary number of integer-order Rényi entropies. This allows for an arbitrary-precision approximation which is relatively computationally cheap, requiring only a sufficient number of integer-order Rényi entropies.

This approximation scheme was developed in the context of quasi-free Fermionic lattice systems for which the Rényi entropy density is well defined. Examples of other, non-linear approximation methods were given, but the main advantage of the scheme introduced in Chapter 2 is linearity. This linearity is crucial since the motivation for this work was in approximating the von Neumann entropy of a system with arbitrary precision in a computationally cheap way.

In Chapter 3, dynamical quantum systems were introduced. As the system of interest evolves in time, so too does its associated entropy. While it is true that closed systems evolve under unitary dynamics, there exists no truly closed system in nature. For open systems, i.e., systems which have some coupling to an uncontrolled environment, the situation is significantly more complex. It is this characterisation of the rate of entropy production in such open systems which is the central focus of Chapters 3 and 4.

Chapter 3 continues by introducing a discrete-time model of an n-level quantum system on a lattice, where shifts along the lattice correspond to discrete time-steps of the underlying (physical) dynamical system. This model is built in such a way that it retains all multi-point correlations for every discrete time-step. The chapter concludes by introducing a means of calculating the average Rényi entropy density for any order, for any quantum system whose dynamics is defined in terms of a completely-positive dynamical map.

Chapter 4 begins by discussing the representation of higher-dimensional tensor structures and their actions on Hilbert space operators. Specifically, care is required in representing the action of composed superoperators on composed operators in order to preserve the correct lexicographical ordering of their elements. Thereafter, the theoretical model introduced in Chapter 3 is applied to a specific example, the qubit which undergoes evolution according to a completely positive Davies map.

Using this modelling technique, it was shown how to optimally adjust the model depending on the dynamics. Once the correct model is defined, the chapter continues by exploring extreme cases, including the classical/Markovian limit and the slow-dissipative limit. The chapter concludes with a numerical example demonstrating the calculation of both the second and third-order average Rényi entropies for a qubit system by picking one particular dynamical map.

The topic of dynamics in general open quantum systems remains a subject of ongoing investigation. Although the modelling technique presented here is rather general, it does make certain assumptions. For example, for practical reasons the dynamics were restricted to Davies maps in Chapter 4. The model itself requires that the dynamics is in terms of some completely positive map and is used to calculate integer-order Rényi entropies.

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List of publications

Journal articles

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